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**Nigel J. Sarginson**
Manager
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ExxonMobil Chemical

***Via Electronic Submission***
e-mail: oppt.ncic@epa.gov, chem.rtk@epa.gov

December 18, 2001



Hon. Christine Todd Whitman
US Environmental Protection Agency
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program

ExxonMobil Chemical Company Registration Number

Dear Ms. Whitman:

ExxonMobil Chemical Company (EMCC) submits for review and public comment the test plan and related robust summaries for the *Olefin Hydroformylation Products* category, under the US High Production Volume (HPV) Chemical Challenge program, AR-201. The test plan and robust summary files are provided electronically in the attached zip file in Word 95/97 format.

This test plan covers the following category of 17 HPV chemicals, Olefin Hydroformylation Products:

CAS# 68527-03-7: Pentene, HOF
CAS# 68938-02-3: Pentene, HOF, low-boiling
CAS# 70955-11-2: Hexene, HOF
CAS# 70955-03-2: Hexene, HOF, low-boiling
CAS# 70955-04-3: Hexene, HOF, high-boiling
CAS# 68526-80-7: Alcohols, C6 and C8 iso, distillation residues
CAS# 68527-04-8: Heptene, HOF
CAS# 68526-96-5: Heptene, HOF, low-boiling
CAS# 68526-88-5: Heptene, HOF, high-boiling
CAS# 68527-05-9: Octene, HOF
CAS# 68526-89-6: Octene, HOF, high-boiling
CAS# 68938-04-5: Nonene, HOF
CAS# 68526-93-2: Nonene, HOF, low-boiling
CAS# 68526-90-9: Nonene, HOF, high-boiling

CAS# 68516-18-7: Decene, HOF
CAS# 68527-06-0: Dodecene, HOF
CAS# 68526-91-0: Dodecene, HOF, high-boiling

Please note that CAS# 68526-80-7: Alcohols, C6 and C8 iso, distillation residues, was not included in our November 12, 1999 commitment letter to the Agency. This chemical was not on the 1990 IUR but was reported by EMCC in the subsequent 1994 IUR update. EMCC now volunteers to sponsor this chemical under the U.S. HPV Challenge program.

We understand that this information will be posted on the internet for a 120 day comment period. Please forward technical comments on this test plan to Laura H. Keller at the above address or you may contact her at (281) 870-6501 (email: laura.h.keller@exxonmobil.com).

Please note that EMCC's corporate contact for future questions from the U.S. EPA about the HPV Challenge Program has been changed from Mr. Gailen A. Hart to:

Mr. Nigel J. Sarginson
ExxonMobil Chemical Company
13501 Katy Freeway
Houston, TX 77079

Phone: (281) 870-6783
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Email: nigel.j.sarginson@exxonmobil.com

Sincerely,

Nigel J. Sarginson
Product Stewardship & Regulatory Affairs Manager
ExxonMobil Chemical Company

Cc: L.H. Keller

AR201-13380A

# HIGH PRODUCTION VOLUME (HPV)

# CHEMICAL CHALLENGE PROGRAM



## ASSESSMENT PLAN

## For The

## OLEFIN HYDROFORMYLATION PRODUCTS CATEGORY

CAS# 68527-03-7: Pentene, HOF
CAS# 68938-02-3: Pentene, HOF, low-boiling
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CAS# 70955-04-3: Hexene, HOF, high-boiling
CAS# 68527-04-8: Heptene, HOF
CAS# 68526-96-5: Heptene, HOF, low-boiling
CAS# 68526-88-5: Heptene, HOF, high-boiling
CAS# 68527-05-9: Octene, HOF
*CAS# 68938-03-4: Octene, HOF, low-boiling
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CAS# 68938-04-5: Nonene, HOF
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*CAS# 68526-92-1: Dodecene, HOF, low-boiling
CAS# 68526-91-0: Dodecene, HOF, high-boiling

* Not an HPV material, included to facilitate category evaluation.

Prepared by:

ExxonMobil Chemical Company

November 29, 2001

# EXECUTIVE SUMMARY

Under the United States Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company has committed to voluntarily compile data for a category of substances defined as olefin hydroformylation products. This category is supported by data for physicochemical, environmental fate and effects, and human health effects endpoints.

ExxonMobil Chemical Company considers the olefin hydroformylation products a category under the HPV Program because their physicochemical and toxicological properties are expected to be very similar and follow a regular pattern as a result of their chemical composition. Products in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These products are residual waste materials remaining from the production of alkyl alcohols, which includes the hydroformylation of pentene, hexene, heptene, octene, nonene, decene, and dodecene. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

The olefins and alkyl alcohols in the olefin hydroformylation products each have a common structure and incrementally increase in carbon number from the lowest to the highest molecular weight product. The structural similarity of chemicals in each of the two groups creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. Because the olefin hydroformylation products are mixtures of alkyl alcohols and their corresponding olefins, combined data from these groups are used to support this test plan. This plan is based on the assumption that the environmental fate and effects, and human toxicological properties of products in the Olefin Hydroformylation Products Category are equivalent to the combined properties of the olefin and respective alcohol. The data for these two groups of products will come from the Alkyl Alcohols C6 - C13 Category and Higher Olefins Category test plans that have been previously submitted under the HPV Program.

The test data compiled for the category anchor studies is adequate to support a screening-level hazard assessment for the Olefin Hydroformylation Products Category and its member products (CAS numbers 68527-03-7, 68938-02-3, 70955-11-2, 68527-04-8, 68527-05-9, 68938-04-5, 68516-18-7, 68527-06-0, 68938-02-3, 70955-03-2, 68526-80-7, 68526-96-5, 68526-93-2, 70955-04-3, 68526-88-5, 68526-89-6, 68526-90-9, 68526-91-0). Member products that lack measured data for selected HPV endpoints can be characterized by extrapolating or interpolating the existing data associated with the component chemicals. For some endpoints, computer modeled data can be used to further support a hazard assessment.

Evaluation of the olefin hydroformylation products as a category has several advantages:

- The data from this category will be used to inform the public about the potential hazards of olefin hydroformylation products.
- Developing a data matrix of anchor studies and applying justifiable read across practices will provide a sufficiently robust data set to characterize each endpoint in the HPV Program without having to conduct a test for each endpoint and product.
- This resourceful use of existing data will result in fewer animals needed for testing purposes while adequately assessing the potential hazards of products in the Olefin Hydroformylation Products Category.

# TABLE OF CONTENTS

# TEST PLAN FOR OLEFIN HYDROFORMYLATION PRODUCTS

## I. INTRODUCTION

Under the United States Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company has committed to voluntarily compile data for a category of substances defined as olefin hydroformylation products. This category is supported by data for physicochemical, environmental fate and effects, and human health effects endpoints.

ExxonMobil Chemical Company considers the olefin hydroformylation products a category under the HPV Program because their physicochemical and toxicological properties are expected to be very similar and follow a regular pattern as a result of their chemical composition. Products in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These products are residual waste materials remaining from the production of alkyl alcohols, which includes the hydroformylation of pentene, hexene, heptene, octene, nonene, decene, and dodecene. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

The olefins and alkyl alcohols in the olefin hydroformylation products each have a common structure and incrementally increase in carbon number from the lowest to the highest molecular weight product. The structural similarity of chemicals in each of the two groups creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. Because the olefin hydroformylation products are mixtures of alkyl alcohols and their corresponding olefins, combined data from these groups are used to support this test plan. This plan is based on the assumption that the environmental fate and effects, and human toxicological properties of products in the Olefin Hydroformylation Products Category are equivalent to the combined properties of the olefin and respective alcohol. The data for these two groups of products will come from the Alkyl Alcohols C6 - C13 Category and Higher Olefins Category test plans that have been previously submitted under the HPV Program.

The test data compiled for the category anchor studies is adequate to support a screening-level hazard assessment for the Olefin Hydroformylation Products Category and its member products (CAS numbers 68527-03-7, 68938-02-3, 70955-11-2, 68527-04-8, 68527-05-9, 68938-04-5, 68516-18-7, 68527-06-0, 68938-02-3, 70955-03-2, 68526-80-7, 68526-96-5, 68526-93-2, 70955-04-3, 68526-88-5, 68526-89-6, 68526-90-9, 68526-91-0). Member products that lack measured data for selected HPV endpoints can be characterized by extrapolating or interpolating the existing data associated with the component chemicals. For some endpoints, computer modeled data can be used to further support a hazard assessment.

Evaluation of the Olefin Hydroformylation Products as a category has several advantages:

- The data from this category will be used to inform the public about the potential hazards of the olefin hydroformylation products.
- Developing a data matrix of anchor studies and applying justifiable read across practices will provide a sufficiently robust data set to characterize each endpoint in the HPV Chemical Challenge Program without having to conduct a test for each endpoint and product.
- This resourceful use of existing data will result in fewer animals needed for testing purposes while adequately assessing the potential hazards of products in the Olefin Hydroformylation Products Category.

## II. CHEMICAL PROCESS AND DESCRIPTION

Products in the Olefin Hydroformylation Products Category are produced by the hydroformylation of pentene, hexene, heptene, octene, nonene, decene, and dodecene. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. The olefin(s) and associated alcohol(s) by carbon number for the CAS numbers in this category are listed in Table 1.

Exposure to Olefin Hydroformylation Products is generally very low since most of the product is recycled and used in feedstocks. Limited quantities have been sold in the United States and Europe for diesel/fuel oil blending. However, since these products are primarily site-limited intermediates, the potential for exposure is quite low.

Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols). Thus, each member of the category is composed of the olefin and corresponding alcohol with an incremental change in carbon number for these components across the category.

The structural similarity of chemicals in each of the two groups creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The compositional features of members of the category are as follows:

- A mix of olefins and alkyl alcohols.
- An incremental increase in carbon number of the olefin and corresponding alkyl alcohol across category members.

**Table 1. CAS Number, Description, and Carbon Number(s) of the Olefin and Corresponding Alcohol for each of the Hydroformylation Products.**

| CAS Number | Product name | Olefin | Alcohol |
|---|---|---|---|
| 68527-03-7 | Pentene, HOF | C5 | C6 |
| 68938-02-3 | Pentene, HOF, low-boiling | C5 | C6 |
| 70955-11-2 | Hexene, HOF | C6 | C7 |
| 70955-03-2 | Hexene, HOF, low-boiling | C6 | C7 |

| CAS Number | Product name | Olefin | Alcohol |
|---|---|---|---|
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | - | C6, C8 |
| 70955-04-3 | Hexene, HOF, high-boiling | - | C7-8 |
| 68527-04-8 | Heptene, HOF | C7 | C8 |
| 68526-96-5 | Heptene, HOF, low-boiling | C7 | C8 |
| 68526-88-5 | Heptene, HOF, high-boiling | - | C8-9 |
| 68527-05-9 | Octene, HOF | C8 | C9 |
| 68938-03-4* | Octene, HOF, low-boiling | C8 | C9 |
| 68526-89-6 | Octene, HOF, high-boiling | - | C9-10 |
| 68938-04-5 | Nonene, HOF | C9 | C10 |
| 68526-93-2 | Nonene, HOF, low-boiling | C9 | C10 |
| 68526-90-9 | Nonene, HOF, high-boiling | - | C10-11 |
| 68516-18-7 | Decene, HOF | C10 | C11 |
| 68527-06-0 | Dodecene, HOF | C12 | C13 |
| 68526-92-1* | Dodecene, HOF, low-boiling | C10-12 | C13 |
| 68526-91-0 | Dodecene, HOF, high-boiling | - | C13-14 |

* Not an HPV material, included to facilitate category evaluation.

Evaluation of the olefin hydroformylation products as a category accomplishes the goal of the Challenge Program - to obtain screening level hazard information - through the strategic evaluation of data for products within this category. The test plan strategy is based on the principle that:

- These products behave in a similar and/or predictable manner, and
- Interpolation and extrapolation of data can be used to characterize the olefin hydroformylation products for which data are not available.

Procedures to assess the reliability of selected studies described in this test plan are based on the guidelines described by Klimisch *et al.*, 1997.

## III. TEST PLAN RATIONALE

### A. Physicochemical Data

Physicochemical data (i.e., melting point, boiling point, vapor pressure, water solubility, and Kow) for selected chemical components in the Olefin Hydroformylation Products Category will be calculated using the EPIWIN© model (EPIWIN, 1999), as discussed in the EPA document titled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." These data will be presented as ranges, based on the chemical components selected to represent each olefin hydroformylation product. In addition, measured data for some of these endpoints will also be provided for selected alcohol and olefin components where readily available. Where possible, the measured and calculated data will be presented together for comparative purposes.

Table 2 lists selected measured physicochemical data (boiling range, vapor pressure, and specific gravity) as they appear on the material safety data sheets for products in this category. These data are provided with this test plan to further justify these products as a distinct category under the HPV Program. As shown by the data in Table

2, the structural similarity within each of the two types of chemicals in the olefin hydroformylation products results in a predictable and incremental pattern of physiochemical properties.

## Table 2. Selected Physical Properties of Olefin Hydroformylation Products

| CAS NUMBER | CHEMICAL NAME | PRIMARY COMPONENTS | BOILING RANGE (° C) | VAPOR PRESSURE (mm Hg @ 100° C) | SPECIFIC GRAVITY | WATER SOLUBILITY (mg/L)* |
|---|---|---|---|---|---|---|
| 68527-03-7 | Pentene, HOF | **C6 Alcohol** | 152-163 | 124 | 0.82 | 10,340-11,950 |
| | | **C5 Olefin** | 44-54 | 506-635 | 0.65 | 210-245 |
| 68938-02-3 | Pentene, HOF, low-boiling | **C6 Alcohol** | 152-163 | 124 | 0.82 | 10,340-11,950 |
| | | **C5 Olefin** | 44-54 | 506-635 | 0.65 | 210-245 |
| 70955-11-2 | Hexene, HOF | **C7 Alcohol** | 167-176 | 78 | 0.83 | 3,539-11,950 |
| | | **C6 Olefin** | 63-73 | 143 | 0.69 | 47-76 |
| 70955-03-2 | Hexene, HOF, low-boiling | **C7 Alcohol** | 167-176 | 78 | 0.83 | 3,539-11,950 |
| | | **C6 Olefin** | 63-73 | 143 | 0.69 | 47-76 |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | **C6,C8 Alcohol** | 152-193 | 27-124 | 0.82-0.83 | 1,379-11,950 |
| | | - | - | - | - | - |
| 70955-04-3 | Hexene, HOF, high-boiling | **C7-C8 Alcohol** | 167-193 | 27-78 | 0.83 | 1,379-11,950 |
| | | - | - | - | - | - |
| 68527-04-8 | Heptene, HOF | **C8 Alcohol** | 185-193 | 27 | 0.83 | 1,379-1,485 |
| | | **C7 Olefin** | 85-100 | 45 | 0.72 | 16.9-33.8 |
| 68526-96-5 | Heptene, HOF, low-boiling | **C8 Alcohol** | 185-193 | 27 | 0.83 | 1,379-1,485 |
| | | **C7 Olefin** | 85-100 | 45 | 0.72 | 16.9-33.8 |
| 68526-88-5 | Heptene, HOF, high-boiling | **C8-C9 Alcohol** | 185-215 | 16-27 | 0.83-0.84 | 164-1,485 |
| | | - | - | - | - | - |
| 68527-05-9 | Octene, HOF | **C9 Alcohol** | 203-215 | 16 | 0.84 | 164-614 |
| | | **C8 Olefin** | 110-116 | 30 | 0.73 | 1.0-5.9 |
| 68938-03-4 | Octene, HOF, low-boiling | **C9 Alcohol** | 203-215 | 16 | 0.84 | 164-614 |
| | | **C8 Olefin** | 110-116 | 30 | 0.73 | 1.0-5.9 |
| 68526-89-6 | Octene, HOF, high-boiling | **C9-C10 Alcohol** | 203-224 | 8.2-16 | 0.84 | 75.0**-614 |
| | | - | - | - | - | - |
| 68938-04-5 | Nonene, HOF | **C10 Alcohol** | 217-224 | 8.2 | 0.84 | 75.0** |
| | | **C9 Olefin** | 135-146 | 5.2 | 0.74 | 0.7-1.5 |
| 68526-93-2 | Nonene, HOF, low-boiling | **C10 Alcohol** | 217-224 | 8.2 | 0.84 | 75.0** |
| | | **C9 Olefin** | 135-146 | 5.2 | 0.74 | 0.7-1.5 |
| 68526-90-9 | Nonene, HOF, high-boiling | **C10-C11 Alcohol** | 217-241 | 3.8-8.2 | 0.84 | 28.0-75.0 |
| | | - | - | - | - | - |
| 68516-18-7 | Decene, HOF | **C11 Alcohol** | 229-241 | 3.8 | 0.84 | 28.0** |
| | | **C10 Olefin** | 163-172 | 1.6 | 0.74 | 1.0 |
| 68527-06-0 | Dodecene, HOF | **C13 Alcohol** | 256-266 | 2.7 | 0.84 | 5.8** |
| | | **C12 Olefin** | 204-214 | 0.2 | 0.76 | 0.1 |
| 68526-92-1 | Dodecene, HOF, low-boiling | **C13 Alcohol** | 256-266 | 2.7 | 0.84 | 5.8** |
| | | **C10-C12 Olefin** | 163-214 | 0.2-1.6 | 0.74-0.76 | 0.1-1.0 |
| 68526-91-0 | Dodecene, HOF, high-boiling | **C13-C14 Alcohol** | 275-310*** | 0.3*** | 0.84*** | 0.8*** |
| | | - | - | - | - | - |

* Calculated using EPIWIN
** Measured values (Robust summaries are attached)
*** Read across values from a C13-C15 alcohol

## B. Human Health Effects

The structural and compositional similarity of the olefin hydroformylation products influences both their physicochemical (Table 2) and their toxicological properties (Table 4). Since olefin hydroformylation products are mixtures of alkyl alcohols and higher olefins, their toxicity can be assessed by evaluating the existing data on alkyl alcohols and higher olefins. As a chemical category, the olefin hydroformylation products, have predictable, low-level environmental and health hazards.

ExxonMobil Chemical Company believes the category of olefin hydroformylation products is scientifically justifiable and that the test data compiled for the category proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers 68527-03-7, 68938-02-3, 70955-11-2, 68527-04-8, 68527-05-9, 68938-04-5, 68516-18-7, 68527-06-0, 68938-02-3, 70955-03-2, 68526-80-7, 68526-96-5, 68526-93-2, 70955-04-3, 68526-88-5, 68526-89-6, 68526-90-9, 68526-91-0). One can assess the untested endpoints by interpolation between and among the category members.

The alcohol component of the olefin hydroformylation products would likely be broken down by mitochondrial beta-oxidation or by cytochrome P450 mediated omega and omega-minus-one oxidation (may be followed by beta-oxidation). The alcohol undergoes various oxidative steps to yield other alcohols, ketones, aldehydes, carboxylic acids and carbon dioxide (Mann, 1987). Data for monohydric, aliphatic alcohols show a systematic variation according to molecular weight in a manner similar to many other homologous series (Monick, 1968). The body handles aliphatic hydrocarbons in a similar manner via oxidative conversion to alcohols, ketones, and eventual elimination as carbon dioxide and carboxylic acids (Wislocki et al, 1980). The undegraded alcohols can be conjugated either directly or as a metabolite with glucuronic acid, sulfuric acid, or glycine and are rapidly excreted (Lington and Bevan, 1994). Intermediate aldehydes could be reactive and bind with DNA and/or proteins. Glucuronidation and glutathione conjugation are possible means of rapid elimination (Mann, 1987).

Table 3 summarizes the data available for the components of each product and the read across strategy applied to the data gaps. Table 4 summarizes the available data used to characterize the toxicity of the olefin hydroformylation products.

## Table 3. Olefin Hydroformylation Products Data Matrix For Mammalian Toxicity Studies

| Olefin Hydroformylation Product | | Component | | Acute Toxicity | Genotox. Point Mutation | Genotox. Chrom. Aberr. | Subchronic Toxicity** | Developmental Toxicity** |
|---|---|---|---|---|---|---|---|---|
| CAS # | Product name | Alcohol | Olefin | Oral | Ames | M. Micron. | | |
| 68527-03-7 | Pentene, HOF | C6 | C5 | A | RA | RA | A | A |
| 68938-02-3 | Pentene, HOF, low-boiling | C6 | C5 | A | RA | RA | A | A |
| 70955-11-2 | Hexene, HOF | C7 | C6 | A | O | O | RA | T(O) |
| 70955-03-2 | Hexene, HOF, low-boiling | C7 | C6 | A | O | O | RA | T(O) |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | C6, C8 | - | A | A | A | A | A |
| 70955-04-3 | Hexene, HOF, high-boiling | C7-C8 | - | A | RA | RA | A | A |
| 68527-04-8 | Heptene, HOF | C8 | C7 | A,O* | A | A,O | A | A |
| 68526-96-5 | Heptene, HOF, low-boiling | C8 | C7 | A,O* | A | A,O | A | A |
| 68526-88-5 | Heptene, HOF, high-boiling | C8-C9 | - | A | A | A | A | A |
| 68527-05-9 | Octene, HOF | C9 | C8 | A,O | RA | RA | A | A |
| 68938-03-4 | Octene, HOF, low-boiling | C9 | C8 | A,O | RA | RA | A | A |
| 68526-89-6 | Octene, HOF, high-boiling | C9-C10 | - | A | RA | RA | A | A |
| 68938-04-5 | Nonene, HOF | C10 | C9 | H,A,O | O | O | RA | A |
| 68526-93-2 | Nonene, HOF, low-boiling | C10 | C9 | H,A,O | O | O | RA | A |
| 68526-90-9 | Nonene, HOF, high-boiling | C10-C11 | - | H,A | RA | RA | A | A |
| 68516-18-7 | Decene, HOF | C11 | C10 | H,A | RA | RA | A | A |
| 68527-06-0 | Dodecene, HOF | C13 | C12 | A,O | A | RA | A | RA |
| 68526-92-1 | Dodecene, HOF, low-boiling | C13 | C10-C12 | A,O | A | RA | A | T(O) |
| 68526-91-0 | Dodecene, HOF, high-boiling | C13-C14 | - | A | A | RA | A | RA |

**A: Data comes from the corresponding alcohol;** Studies are reliable (Robust Summaries presented).
**O: Data comes from the corresponding olefin;** Studies are reliable (Robust Summaries presented).
**H: Data is on the hydroformylation mixture**; Studies are reliable (Robust Summaries presented).
**RA** Read Across Extrapolation. T(O): Testing proposed in ACC Higher Olefins Test Plan. O*: Acute dermal data.
** Reproductive toxicity will be assessed by read-across to Developmental Toxicity Studies and Repeat Dose Toxicity Studies that included histopathology on male and female sex organs and accessory sex organs.

# Table 4. Summary of Toxicology Data for Olefin Hydroformylation Products

| Olefin Hydroformylation Product | | Acute Toxicity | Genotox. Point Mutation | Genotox. Chrom. Aberr. | Subchronic Toxicity** NOAEL | Developmental Toxicity** NOAEL |
|---|---|---|---|---|---|---|
| CAS # | Product name | Oral (Dermal) | Ames | M. Micron. | | |
| 68527-03-7 | Pentene, HOF | | | | | |
| | C6Alcohol | 3.7 g/kg (>2.6 g/kg) | RA | RA | =0.5% in diet (rat, dog) = 2.0 mg/kg/day (rat, dermal) | Inhal: Dam/Pup = 3500 mg/m$^3$ |
| | C5 Olefin | RA | RA | RA | RA | RA |
| 68938-02-3 | Pentene, HOF, low-boiling | | | | | |
| | C6Alcohol | 3.7 g/kg (>2.6 g/kg) | RA | RA | =0.5% in diet (rat, dog) = 2.0 mg/kg/day (rat, dermal) | Inhal: Dam/Pup = 3500 mg/m$^3$ |
| | C5 Olefin | RA | RA | RA | RA | RA |
| 70955-11-2 | Hexene, HOF | | | | | |
| | C7 Alcohol | =3.9 g/kg (> 3.2 g/kg) | RA | RA | RA | RA |
| | C6 Olefin | RA | Negative | Negative | RA | T (C6 Olefin) |
| 70955-03-2 | Hexene, HOF, low-boiling | | | | | |
| | C7 Alcohol | =3.9 g/kg (> 3.2 g/kg) | RA | RA | RA | RA |
| | C6 Olefin | RA | Negative | Negative | RA | T (C6 Olefin) |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | | | | | |
| | C6, C8 Alcohol | 3.7 g/kg (>2.6 g/kg) | Negative (2-ethyl-1-hexanol) | Negative (2-ethyl-1-hexanol) | =0.5% in diet (rat, dog) = 2.0 mg/kg/day (rat, dermal) | Inhal: Dam/Pup = 3500 mg/m$^3$ |
| | - | - | - | - | - | - |
| 70955-04-3 | Hexene, HOF, high-boiling | | | | | |
| | C7-C8 Alcohol | =3.9 g/kg (> 3.2 g/kg) | RA | RA | = 2.0 mg/kg/day (rat, dermal)<br>=130 mg/kg/day (rat)<br>NOEL = 125 mg/kg/day (LOEL = 250 mg/kg/day) (rat) | Dam: 500 mg/kg/day Pup: 1000 mg/kg/day Inhal: Dam/Pup 400 mg/m$^3$ |
| | - | - | - | - | - | - |

## Table 4. Continued

| Olefin Hydroformylation Product | | Acute Toxicity | Genotox Point Mutations | Genotox Chrom. Aber. | Subchronic Toxicity** NOAEL | Developmental Toxicity** NOAEL |
|---|---|---|---|---|---|---|
| 68527-04-8 | Heptene, HOF | | | | | |
| | C8 alcohol | > 2.0 g/kg (> 2.6 g//kg) | Negative (2-ethyl-1-hexanol) | Negative (2-ethyl-1-hexanol) | = 2.0 mg/kg/day (rat, dermal)<br>=130 mg/kg/day (rat)<br>NOEL = 125 mg/kg/day (LOEL = 250 mg/kg/day) (rat) | Dam: 500 mg/kg/day<br>Pup: 1000 mg/kg/day<br>Inhal: Dam/Pup 400 $mg/m^3$ |
| | C7 Olefin | RA (> 3.2 g/kg) | RA | Negative | RA | RA |
| 68526-96-5 | Heptene, HOF, low-boiling | | | | | |
| | C8 Alcohol | > 2.0 g/kg (> 2.6 g//kg) | Negative (2-ethyl-1-hexanol) | Negative (2-ethyl-1-hexanol) | = 2.0 mg/kg/day (rat, dermal)<br>=130 mg/kg/day (rat)<br>NOEL = 125 mg/kg/day (LOEL = 250 mg/kg/day) (rat) | Dam: 500 mg/kg/day<br>Pup: 1000 mg/kg/day<br>Inhal: Dam/Pup 400 $mg/m^3$ |
| | C7 Olefin | RA (> 3.2 g/kg) | RA | Negative | RA | RA |
| 68526-88-5 | Heptene, HOF, high-boiling | | | | | |
| | C8-C9 Alcohol | > 2.0 g/kg (> 2.6 g//kg) | Negative (2-ethyl-1-hexanol) | Negative (2-ethyl-1-hexanol) | =130 mg/kg/day | Dam: 500 mg/kg/day<br>Pup: 1000 mg/kg/day<br>Inhal: Dam/Pup 400 $mg/m^3$ |
| | - | - | - | - | - | - |
| 68527-05-9 | Octene, HOF | | | | | |
| | C9 Alcohol | = 3.0 g/kg (> 3.2 g/kg) | RA | RA | = 144 mg/kg/day | Dam: 144 mg/kg/day<br>Pup: 144 mg/kg/day |
| | C8 Olefin | > 5.0 g/kg (> 3.2 g/kg) | RA | RA | RA | RA |
| 68938-03-4 | Octene, HOF, low-boiling | | | | | |
| | C9 Alcohol | = 3.0 g/kg (> 3.2 g/kg) | RA | RA | = 144 mg/kg/day | Dam: 144 mg/kg/day<br>Pup: 144 mg/kg/day |
| | C8 Olefin | > 5.0 g/kg (> 3.2 g/kg) | RA | RA | RA | RA |
| 68526-89-6 | Octene, HOF, high-boiling | | | | | |
| | C9-C10 Alcohol | = 3.0 g/kg (> 3.2 g/kg) | RA | RA | = 144 mg/kg/day | Dam: 158 mg/kg/day<br>Pup: 790 mg/kg/day |
| | - | - | - | - | - | - |

## Table 4. Continued

| Olefin Hydroformylation Product | | Acute Toxicity | Genotox. Point Mutation | Genotox. Chrom. Aber. | Subchronic Toxicity** NOAEL | Developmental Toxicity** NOAEL |
|---|---|---|---|---|---|---|
| 68938-04-5 | Nonene, HOF | > 5.0 g/kg (> 3.2 g/kg) | | | | |
| | C10 Alcohol | = 4.6 g/kg | RA | RA | RA | Dam: 158 mg/kg/day Pup: 790 mg/kg/day |
| | C9 Olefin | > 2.3 g/kg (> 2.3 g/kg) | Negative | Negative | RA | RA |
| 68526-93-2 | Nonene, HOF, low-boiling | > 5.0 g/kg (> 3.2 g/kg) | | | | |
| | C10 Alcohol | = 4.6 g/kg | RA | RA | RA | Dam: 158 mg/kg/day Pup: 790 mg/kg/day |
| | C9 Olefin | > 2.3 g/kg (> 2.3 g/kg) | Negative | Negative | RA | RA |
| 68526-90-9 | Nonene, HOF, high-boiling | > 5.0 g/kg (> 3.2 g/kg) | | | | |
| | C10-C11 Alcohol | = 4.6 g/kg (> 2.6 g/kg) | RA | RA | 100 mg/kg/day | Dam: 158 mg/kg/day Pup: 790 mg/kg/day |
| | - | - | - | - | - | - |
| 68516-18-7 | Decene, HOF | > 5.0 g/kg (> 3.2 g/kg) | | | | |
| | C11 Alcohol | = 4.6 g/kg (> 2.6 g/kg) | RA | RA | 100 mg/kg/day | Dam/Pup: > 1,440 mg/kg/day |
| | C10 Olefin | RA | RA | RA | RA | RA |
| 68527-06-0 | Dodecene, HOF | | | | | |
| | C13 Alcohol | > 2.0 g/kg | Negative (1-dodecanol) | RA | = 100 mg/kg/day | RA |
| | C12 Olefin | > 7.7 g/kg (> 2.5 g/kg) | RA | RA | RA | RA |
| 68526-92-1 | Dodecene, HOF, low-boiling | | | | | |
| | C13 Alcohol | > 2.0 g/kg | Negative (1-dodecanol) | RA | = 100 mg/kg/day | RA |
| | C10-C12 Olefin | > 7.7 g/kg (> 2.5 g/kg) | RA | RA | RA | T (C18 Olefin) |
| 68526-91-0 | Dodecene, HOF, high-boiling | | | | | |
| | C13-C14 Alcohol | > 2.0 g/kg | Negative (1-dodecanol) | RA | = 100 mg/kg/day | RA |
| | - | - | - | - | - | - |

**RA** Read Across Extrapolation.

** Reproductive toxicity will be assessed by read-across to Developmental Toxicity Studies and Repeat Dose Toxicity studies that included histopathology on male and female sex organs and accessory sex organs.

T: Test proposed in ACC Higher Olefins test plan.

## C. Presentation of Olefin Hydroformylation Products Category Data Associated with the Anchor Studies under the HPV Challenge Program

### Acute Oral Toxicity

All of the olefin hydroformylation products have a low order of toxicity to rats via the oral route of exposure based on data from the hydroformylation products themselves as well as data from the corresponding alkyl alcohols and higher olefins (Table 4). The $LD_{50}$ for the hydroformylation products is greater than 5.0 g/kg. The $LD_{50}$ for the C6 branched and linear alkyl alcohol anchor study was >3.7 g/kg (Scala, 1973). The $LD_{50}$'s for the C6-C8, C7-C9, C8-C10, C9-C11, and C11-C14 branched alkyl alcohols were all > 2 g/kg. For all of the alkyl alcohols, acute oral exposure induced signs of systemic toxicity that were characterized by depression, sedation, and ataxia. These results demonstrate that members of the alkyl alcohol category have a consistent, low order of acute oral toxicity. The higher olefins also have a low order of acute toxicity. For all of the higher olefins, the $LD_{50}$ was at least greater than 2.3 g/kg. Taken together, the acute toxicity data for the alkyl alcohols and the higher olefins demonstrates that the olefin hydroformylation products have a low order of acute toxicity.

### Acute Dermal Toxicity

The Olefin hydroformylation products have a low order of toxicity via the dermal route of exposure based on data from the hydroformylation products themselves as well as the component alkyl alcohols and olefins (Table 4). The dermal $LD_{50}$ for all of the hydroformylation products was greater than 3.2 g/kg. The rabbit dermal $LD_{50}$ for all of the alkyl alcohols was greater than 2.6 g/kg. This indicates that the members of this category have a consistent pattern of acute toxicity via the dermal route of exposure.

### Genotoxicity

***In Vitro***:
Based on mutagenicity data for alkyl alcohols and higher olefins, Olefin hydroformylation products are not considered mutagenic (Table 4). The weight of evidence from this existing data supports the conclusion that these materials are not genotoxic and obviates the need for further testing.

***Mutagenicity data on alcohol components:***
Existing data on 1-hexanol, which is an isomer of Alkyl Alcohol C6, indicates that this material is not genotoxic. Although a robust summary for this study is not provided, the summary is available in IUCLID (ECBa). In addition, 2-ethyl-1-hexanol and 1-dodecanol were evaluated in Ames assays in the presence and absence of metabolic activation. The 2-ethyl-1-hexanol is an isomer of Alkyl Alcohol C7-C9, and the 1-dodecanol is an isomer of Alkyl Alcohol C11-C14. Both materials were not mutagenic in Ames assays using five strains of *Salmonella typhimurium.*

Additional data to support the assessment of mutagenicity comes from the alkyl acetates, which are metabolized to the corresponding alkyl alcohol. The members of this category have been extensively evaluated for mutagenicity and have been shown to

be non-mutagenic (EMCCa). For further details on the assessment of the mutagenicity of alkyl alcohols, please refer to the EMCC Test Plan for Alkyl Alcohols (EMCCb).

***Mutagenicity data on higher olefin components:***
Higher olefins have been evaluated for mutagenicity in Ames assays. Both $C_6$ and $C_9$ olefins were evaluated in Ames assays in the presence and absence of metabolic activation. Both materials produced negative results, indicating that they are not mutagenic. In addition, bacterial mutagenicity studies on larger molecular weight higher olefins, i.e. C20-24 higher olefins, indicate that the higher molecular weight olefins are also not mutagenic. Robust summaries for these studies are available through the ACC Higher Olefins Test Plan (ACC, 2001).

All together, the weight of evidence demonstrates that olefin hydroformylation products are not mutagenic as shown by the negative mutagenicity data on the alcohols and higher olefins.

***In Vivo***
Based on existing data for alkyl alcohols, higher olefins, and structurally similar materials, members of the Olefin Hydroformylation Products Category are not considered to be clastogenic (Table 4). Existing data in addition to data forthcoming from the Alkyl Alcohols Testing Program will be used to evaluate the clastogenicity of the olefin hydroformylation products.

***Clastogenicity data on the alcohols:***
A detailed assessment of the clastogenicity of the alkyl alcohols and the proposed testing is presented in the EMCC Test Plan for Alkyl Alcohols (EMCCb) that has been submitted to the US EPA. The assessment is based on existing data for structural isomers of the alkyl alcohols, existing data on metabolic precursors, and forthcoming data on proposed testing for the category. In short, the existing data for structural isomers comes from mouse micronucleus studies on 2-ethyl-1-hexanol (ECBc) and 1-dodecanol (ECBb) and mouse lymphoma studies on 2-ethyl-1-hexanol. The alkyl acetates, as mentioned above, are metabolic precursors to the alkyl alcohols and produced negative results in mouse micronucleus assays (EMCCa). Together, these data demonstrate a consistent pattern of toxicity for the alkyl alcohols and obviates the need for extensive clastogenicity testing of these materials. To complete the category evaluation of the alkyl alcohols, a mouse micronucleus test on the $C_6$ alkyl alcohol (CAS # 68526-79-4) has been proposed. The results of this test will be compared with the data already available to evaluate the clastogenicity of alkyl alcohols. The forthcoming data from this testing program will be used to complete the assessment of the clastogenicity of olefin hydroformylation products. This strategy will also address animal welfare concerns by reducing the number of animals required to evaluate the category.

***Clastogenicity data on higher olefins:***
In addition to the negative clastogenicity data for alcohols, studies conducted on higher olefins also indicate that these materials are not clastogenic. Both a C6 and a C9 higher olefin have been evaluated in Ames studies with 5 strains of *Salmonella typhimurium* in the presence and absence of metabolic activation. The results of these tests were negative. These materials as well as a C7 higher olefin were also evaluated

for their ability to induce chromosome aberrations in a mouse micronucleus assay. The C6 higher olefin produced a weakly positive response at the highest dose (5 g/kg) when administered by oral gavage. However, when the material was evaluated in the mouse micronucleus assay following inhalation exposure, the most relevant route of exposure, it produced negative results. Given that the C6 higher olefin was not genotoxic in the Ames test or in the micronucleus test when administered by inhalation and given the very slight response seen in the oral micronucleus assay, the C6 higher olefin is not considered to be genotoxic.

Two other higher olefins, the C7 and C9 olefins also produced negative results in the mouse micronucleus assay. In addition, data from *in vitro* cytogenicity and mouse micronucleus tests on larger molecular weight higher olefins, i.e. C20-24 higher olefins, indicate that the higher molecular weight olefins are also not clastogenic. Robust summaries for these studies are available through the ACC Higher Olefins Test Plan (ACC, 2001). Hence, the weight of evidence shows that the higher olefins are not clastogenic.

In summary, olefin hydroformylation products are not considered clastogenic based on existing data for the alcohols and higher olefins. Additional data produced in the EMCC Alkyl Alcohols testing program can be used to provide further support for this category assessment. Importantly, this strategy will reduce the amount of unnecessary animal testing.

**Subchronic Toxicity**

As with the previous endpoints, the subchronic toxicity of olefin hydroformylation products will be assessed from the data on alkyl alcohols and higher olefins (Table 4).

***Subchronic toxicity data on alcohols:***
An evaluation of the repeated dose studies for alkyl alcohols indicates that olefin hydroformylation products have a low order of subchronic toxicity.

A 14-week oral subchronic study was conducted in rats with C11-C14 branched alkyl alcohols at doses of 0, 100, 500, and 1000 mg/kg/day of body weight administered by gavage. At the mid and high-dose levels, females did not display any differences in body weight or food consumption, but had significantly higher mean platelet counts compared to controls. In contrast, males had significantly lower body weights and food consumption, however, hematological parameters were within normal ranges. At the middle and high doses, males and females had significantly higher liver weights than animals in the control group. In addition, males of the high dose group had higher relative brain and testes weights relative to the controls while relative adrenal weight was increased in the high dose females. There were no pathological findings in these tissues, and the organ weight changes were most likely either adaptive responses or merely a consequence of the body weight effects. No other treatment-related weight or histopathological changes were observed in the other organs, including female reproductive organs. The significance of these subtle changes on hematological parameters is unknown, but like the organ weight differences, occurred only after repeat

administration of extremely high doses of Alkyl Alcohols C11-C14 by oral gavage. The NOAEL of this study was 100 mg/kg/day.

Subchronic toxicity data on 1-hexanol, an isomer of Alkyl Alcohol C6, indicates that this material has a low order of subchronic toxicity. Thirteen-week dietary feeding studies in both the rat and dog produced a NOAEL greater than or equal to 0.5% in the diet. Furthermore, a number of studies have evaluated the toxicity of repeated exposure to 2-ethylhexanol, an isomer of Alkyl Alcohol C7-9. In a 3-month study in rats, 2-ethylhexanol was administered by oral gavage at doses of 25, 125, 250, and 500 mg/kg/day. At the highest doses (250 and 500 mg/kd/day), changes in body and organ weights were observed. The NOEL for the study was 125 mg/kg/day and the LOEL for the study was 250 mg/kg/day based on body weight changes. Summaries of the subchronic studies on 1-hexanol and 2-ethylhexanol are publicly available from the European Chemicals Bureau (ECB) IUCLID database and are included with this submission (ECB, 2000).

A 14-day oral study was conducted in Wistar rats with iso-octanol and isononanol at doses of 130 mg/kg/day and 144 mg/kg/day, respectively. Plasma cholesterol and triglycerides were analyzed, the testes and liver were weighed, and the liver was analyzed for both histopathological lesions and the activity of peroxisomal enzymes. No treatment-related effects were observed during the study. Neither iso-octanol nor isononanol induced any significant changes in testes or liver weight, vacuolation, or activity of the peroxisome-associated enzymes. The NOAEL for iso-octanol was the limit dose of 130 mg/kg/day and the NOAEL for isononanol was the limit dose of 144 mg/kg/day.

Dermal exposure of rats to 0.4 and 2.0 mg/kg/day hexyl alcohol or Alkyl alcohol C7 - 9, branched for 10 days resulted in no clinical signs of toxicity at any time during the study. All animals survived to study termination and there were no treatment-related clinical, in-life, gross postmortem or microscopic findings. The no observable adverse effect level (NOAEL) for repeat dermal exposure was 2.0 mg/kg/day.

Taken together, the results of these studies demonstrate that Alkyl Alcohols C6-C13 have a low order or toxicity under conditions of repeat exposure by both the oral and dermal routes. In addition, they demonstrate that the members of the category display a consistent degree of subchronic toxicity by either the oral or dermal routes of exposure. Given that olefin hydroformylation products are composed of alkyl alcohols, these data indicate that they have a low order of subchronic toxicity.

***Subchronic toxicity data on higher olefins:***
Currently, there are no data to assess the subchronic toxicity of the lower molecular weight higher olefins. However, subchronic toxicity data on a C6 higher olefin is forthcoming through the ACC Higher Olefins Panel (ACC, 2001). In the spirit of reducing unnecessary animal testing and because higher olefins are a component of Olefin Hydroformylation Products, the data from this testing program will support an assessment of the Olefin Hydroformylation Products.

Data from subchronic tests of a higher molecular weight olefin, i.e. C20-24, indicate that these materials have a low order of toxicity in 13-week studies (NOAEL = 1000 mg/kg/day). A robust summary of this data is available through the ACC Higher Olefins Test Plan (ACC, 2001). This data and the forthcoming test data for the C6 olefin will be used to evaluate the subchronic toxicity of the Olefin Hydroformylation Products. Therefore, no subchronic toxicity testing is proposed for the olefin hydroformylation products, as this would be redundant. Furthermore, existing data on the alkyl alcohols demonstrate that olefin hydroformylation products have a low order of toxicity under conditions of repeat exposure by both the oral and dermal routes. In addition, they demonstrate that the members of the category display a consistent degree of subchronic toxicity by either the oral or dermal routes of exposure. Therefore, olefin hydroformylation products do not require further testing to assess subchronic toxicity.

## Developmental Toxicity

Studies on the developmental toxicity of the alkyl alcohol and higher olefin components of the olefin hydroformylation products indicate that these materials have a lower order of toxicity and are not considered selective developmental toxicants by either the oral or inhalation routes of exposure (Table 4).

### *Developmental toxicity studies on alcohols:*

### Oral Exposure

Studies on the developmental toxicity of Alkyl Alcohols C6-C13 indicate that these materials have a low order of toxicity and are not considered selective developmental toxicants by either the oral or inhalation routes of exposure. Alkyl alcohol C7-9, branched was orally administered at 100, 500, and 1000 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen in the high dose group as indicated by emaciation, rales, and hypoactivity. However, no adverse maternal effects were observed in the low or mid-dose groups. In addition, there were no significant signs of fetal toxicity in any of the dose groups. A maternal NOAEL of 500 mg/kg and a fetal NOAEL of 1000 mg/kg were observed.

In another study, the developmental toxicity of isononylalcohol 1 and isononylalcohol 2 were evaluated in Wistar rats. Isononylalcohol 1 consists of isomers with a moderate degree of branching (dimethyl heptanols) and contains approximately 16% isodecanol. Isononylalcohol 2 consists of isomers with a low degree of branching (dimethyl heptanols and methyl octanols). Each test substance was administered by oral gavage at 144, 720, or 1440 mg/kg/day during days 6-15 of gestation. At the middle and high dose levels of isononylalcohol 1, signs of maternal and fetal toxicity, including decreased body weight, were observed. At the lowest dose of isononylalcohol 1, no maternal toxicity was observed. There were an increased number of fetuses with hydroureter. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. Therefore, isononylalcohol 1 was considered to induce developmental toxicity only at doses that induce overt maternal toxicity. Isononylalcohol 2 also produced maternal and fetal effects at both the middle and high doses. At the lowest dose however, no maternal or fetal toxicity was observed.

Therefore, isononylalcohol 2 induced fetal toxicity at doses that also induce overt maternal toxicity. The maternal NOAEL for isononylalcohol 1 and isononylalcohol 2 is 144 mg/kg. The fetal NOAEL for isononylalcohol 1 is less than 144 mg/kg, whereas the fetal NOAEL for isononylalcohol 2 is 144 mg/kg.

In a similar study, the developmental toxicity of isodecanol (isomers of trimethyl heptanols and dimethyl octanols) was evaluated in Wistar rats by oral gavage at doses of 158, 790, and 1580 mg/kg during days 6-15 of gestation. Signs of compound-induced toxicity including reduced body weight were observed in dams of the middle and high dose groups. No maternal signs of toxicity were observed in the low dose group. Fetotoxic effects including reduced mean fetal body weight and skeletal retardations were observed only in the highest dose group. The maternal NOAEL for this study was 158 mg/kg and the fetal NOAEL was 790 mg/kg. Thus, isodecanol is fetotoxic only at doses that produce overt maternal toxicity.

An identical study conducted concurrently on C-7-9-11 alcohol (consists of isomers of heptanol, nonanol, and undecanol) produced negative results at all three dose levels tested: 144, 720, and 1440 mg/kg/day. No adverse effects were observed in dams or in the fetuses at any of these doses. The NOAEL for this study was therefore 1440 mg/kg/day.

**Inhalation Exposure**

The developmental toxicity resulting from inhalation of saturated vapors has also been evaluated for several members of the Alkyl Alcohols C6 - C13 category. Inhalation of Alkyl Alcohols C6-C13 is the primary concern during industrial use, particularly for the lower molecular weight members of the category. Therefore, an evaluation of inhalation studies is useful for evaluating the developmental toxicity of the category.

The available developmental toxicity data for structural isomers of the Alkyl Alcohols indicate that these materials are not developmentally toxic via the inhalation route of exposure. Inhalation of saturated vapors of 1-hexanol (3500 mg/m$^3$) resulted in no significant signs of maternal or fetal toxicity. The NOAEL for both maternal and fetal effects for this study was the limit dose of 3500 mg/m$^3$.

Another study evaluated the developmental toxicity of three structurally related alcohols, 1-octanol, 1-nonanol, and 1-decanol following inhalation. Sprague-Dawley rats were exposed to saturated vapors of 1-octanol (400 mg/m$^3$), 1-nonanol (150 mg/m$^3$), and 1-decanol (100 mg/m$^3$) for 7 hours per day during days 1-19 of gestation. No significant effects, including no changes in maternal weight gain, feed consumption, or water intake were observed between the control and any of the treated groups. In addition, no fetal toxicity was observed, as indicated by fetal body weight, sex ratio, and the number of resorptions. The NOAEL for both maternal and fetal effects for each test substance was the saturated vapor concentration: 1-octanol (400 mg/m$^3$, 1-nonanol (150 mg/m$^3$), and 1-decanol (100 mg/m$^3$).

Collectively, the weight of evidence demonstrates that Alkyl Alcohols C6-C13 have a low order or maternal toxicity and do not induce signs of developmental toxicity until maternal toxicity is observed. Hence, these materials are not selective developmental

toxicants. In addition, the maternal and fetal NOAELs for oral exposure to different members of the category are consistent. Furthermore, the NOAELs for inhalation reflect the maximum achievable vapor concentration. Since these materials are not selective toxicants and display a consistent, low order of developmental toxicity they will not undergo further testing for developmental toxicity.

Collectively, the weight of evidence for alkyl alcohols demonstrates that olefin hydroformylation products have a low order or maternal toxicity and do not induce signs of developmental toxicity until maternal toxicity is observed. Hence, these materials are not selective developmental toxicants. In addition, the maternal and fetal NOAELs for oral exposure to different members of the category are consistent, indicating that there are no major differences in the potency of the category members. The NOAELs for developmental toxicity from inhalation reflect the maximum achievable vapor concentration of each test substance. However, in all cases, the NOAEL exceeded the maximum achievable vapor concentration. Since these materials are not selective toxicants and display a consistent, low order of developmental toxicity they will not undergo further testing for developmental toxicity.

***Developmental toxicity of higher olefins:***

Developmental studies on the higher olefins, which are also components of the olefin hydroformylation products, are in progress with the ACC Higher Olefins Panel. A developmental/reproductive/subchronic toxicity screen will be conducted on a C6 olefin and a developmental/reproductive screen will be conducted on a C18 olefin. The data and robust summaries of these tests will be forthcoming under the ACC Higher Olefins test plan.

As discussed above, the existing data for the alcohol component of olefin hydroformylation products demonstrates a consistent pattern of toxicity for the category. The forthcoming data under the ACC Higher Olefins Test Program will provide further support to assess developmental toxicity. By taking this approach, the Olefin Hydroformylation Products Category can be evaluated while the generation of redundant data and unnecessary animal testing is minimized.

**Reproductive Toxicity**

The available developmental toxicity studies and repeat-dose studies prove adequate to support a screening-level hazard assessment for the reproductive toxicity potential of olefin hydroformylation products (Table 4). Developmental toxicity studies conducted by the oral route of exposure on corresponding alkyl alcohols including Isooctyl alcohol, Isononyl alcohol, Isodecanol, and Undecyl alcohol, produced consistent results and demonstrated that these materials do not affect reproductive parameters. Although a slight increase in resorptions was observed in several studies, this only occurred in the highest dose group and in the presence of overt maternal toxicity. Furthermore, inhalation exposure to saturated vapors of 1-hexanol, 1-octanol, 1-nonanol, and 1-decanol did not induce any significant changes in reproductive parameters. In the subacute studies of isooctyl alcohol and isononyl alcohol, no changes in testicular weight were observed. In addition, no histopathological effects in male and female

reproductive organs were observed in the subchronic study conducted on C11-C14 alcohols. These data support the conclusion that the Alkyl Alcohols C6-C13 are not selective reproductive toxicants.

Additional support to evaluate the reproductive toxicity of olefin hydroformylation products is forthcoming from the reproductive toxicity studies proposed in the ACC Higher Olefins Category Test Plan (ACC). To evaluate the reproductive toxicity of the olefin components, a developmental/reproductive/subchronic toxicity screen will be conducted on a C6 olefin and a developmental/reproductive screen will be conducted on a C18 olefin. The data and robust summaries of these tests will be forthcoming under the ACC Higher Olefins test plan.

According to the OECD SIDS Guidelines, adequate developmental toxicology data coupled with subchronic toxicity data that shows no effects on reproductive organs fulfills the requirement for an assessment of reproductive toxicity potential.

## D. Aquatic Toxicity

Aquatic endpoints for the HPV Program include acute toxicity to a freshwater fish and invertebrate, and toxicity to a freshwater alga. The olefin and alkyl alcohol components of products in this category have been shown to produce an expected increasing level of toxicity to freshwater organisms with increasing molecular weight of the product components. This is based on data from the literature that are used to read across to selected components of products in this test plan, data specifically for components of the products in this category, as well as on results of computer modeling using ECOSAR (1999) for selected component chemicals [ECOSAR is an aquatic toxicity modeling program and is a subroutine contained in EPIWIN (1999)].

Table 5 identifies the type of data available for the components of each product and the read across strategy applied to the data gaps. Table 6 summarizes the available data used to characterize the aquatic toxicity of olefin hydroformylation products.

Modeled data consistently correlated well with the experimental data used to characterize acute toxicity for the alcohol and olefin components in this category. This suggests that the ECOSAR model is sufficiently robust to accurately calculate the toxicity of this range of chemicals and can be used to develop reliable toxicity data to complete data gaps.

## Table 5. Olefin Hydroformylation Products Data Matrix for Aquatic Toxicity, Identifying the Type of Data Available for the Components of each Product and the Read Across Strategy Applied to the Data Gaps

| Olefin Hydroformylation Product | | Component | | Fish Acute Toxicity | Invertebrate Acute Toxicity | Alga Toxicity |
|---|---|---|---|---|---|---|
| CAS # | Product Name | Alcohol | Olefin | | | |
| 68527-03-7 | Pentene, HOF | C6 | C5 | A, E | E | E |
| 68938-02-3 | Pentene, HOF, low-boiling | C6 | C5 | A, E | E | E |
| 70955-11-2 | Hexene, HOF | C7 | C6 | A, O | A, E | E |
| 70955-03-2 | Hexene, HOF, low-boiling | C7 | C6 | A, O | A, E | E |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | C6, C8 | - | A | A | E |
| 70955-04-3 | Hexene, HOF, high-boiling | C7-C8 | - | RA | RA | RA |
| 68527-04-8 | Heptene, HOF | C8 | C7 | A, E | A, E | E |
| 68526-96-5 | Heptene, HOF, low-boiling | C8 | C7 | A, E | A, E | E |
| 68526-88-5 | Heptene, HOF, high-boiling | C8-C9 | - | RA | RA | RA |
| 68527-05-9 | Octene, HOF | C9 | C8 | A, O | A, E | A, E |
| 68938-03-4 | Octene, HOF, low-boiling | C9 | C8 | A, O | A, E | A, E |
| 68526-89-6 | Octene, HOF, high-boiling | C9-C10 | - | RA | RA | RA |
| 68938-04-5 | Nonene, HOF | C10 | C9 | A, E | E | E |
| 68526-93-2 | Nonene, HOF, low-boiling | C10 | C9 | A, E | E | E |
| 68526-90-9 | Nonene, HOF, high-boiling | C10-C11 | - | RA | RA | RA |
| 68516-18-7 | Decene, HOF | C11 | C10 | A, O | E | E |
| 68527-06-0 | Dodecene, HOF | C13 | C12 | O | A | RA |
| 68526-92-1 | Dodecene, HOF, low-boiling | C13 | C10-C12 | O | A | RA |
| 68526-91-0 | Dodecene, HOF, high-boiling | C13-C14 | - | RA | RA | RA |

A **Measured data for the alcohol** (study is reliable without restriction; robust summary available).
O **Measured data for the olefin** (study is reliable without restriction; robust summary available).
E Modeled data from ECOSAR for a fish, invertebrate, and/or alga, for the alcohol and/or olefin component.
RA Read Across

## Table 6. Olefin Hydroformylation Products Data Matrix for Aquatic Toxicity, Measured and Modeled Component Data Associated with each Product

| Olefin Hydroformylation Product | | Fish Acute Toxicity 96-hour | Invertebrate Acute Toxicity 48-hour | Alga Toxicity 96-hour |
|---|---|---|---|---|
| CAS # | Product Name | | | |
| 68527-03-7 | Pentene, HOF | | | |
| | C6 Alcohol | **97.7 mg/L**** | 137 mg/L* | 73.2 mg/L* |
| | C5 Olefin | 12.5 mg/L* | 14.0 mg/L* | 9.1 mg/L* |
| 68938-02-2 | Pentene, HOF, low-boiling | | | |
| | C6 Alcohol | **97.7 mg/L** | 137 mg/L* | 73.2 mg/L* |
| | C5 Olefin | 12.5 mg/L* | 14.0 mg/L* | 9.1 mg/L* |
| 70955-11-2 | Hexene, HOF | | | |
| | C7 Alcohol | **34.5 mg/L** | **63 mg/L** | 30.7 mg/L* |
| | C6 Olefin | **6.6 mg/L** | 6.0 mg/L* | 4.0 mg/L* |
| 70955-03-2 | Hexene, HOF, low-boiling | | | |
| | C7 Alcohol | **34.5 mg/L** | **63 mg/L** | 30.7 mg/L* |
| | C6 Olefin | **6.6 mg/L** | 6.0 mg/L* | 4.0 mg/L* |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | | | |
| | C6, C8 Alcohol | **RA** | RA | RA |
| | - | - | - | - |
| 70955-04-3 | Hexene, HOF, High-boiling | | | |
| | C7-C8 Alcohol | RA | RA | RA |
| | - | - | - | - |
| 68527-04-8 | Heptene, HOF | | | |
| | C8 Alcohol | **14.0 mg/L** | **31.8 mg/L** | 12.4 mg/L* |
| | C7 Olefin | 2.1 mg/L* | 2.5 mg/L* | 1.7 mg/L* |
| 68526-96-5 | Heptene, HOF, low-boiling | | | |
| | C8 Alcohol | **14.0 mg/L** | **31.8 mg/L** | 12.4 mg/L* |
| | C7 Olefin | 2.1 mg/L* | 2.5 mg/L* | 1.7 mg/L* |
| 68526-88-5 | Heptene, HOF, high-boiling | | | |
| | C8-C9 Alcohol | RA | RA | RA |
| | - | - | - | - |
| 68527-05-9 | Octene, HOF | | | |
| | C9 Alcohol | **10.1 mg/L** | **4.9 mg/L** | **8.5 mg/L** |
| | C8 Olefin | **0.9 mg/L** | 1.0 mg/L* | 0.7 mg/L* |
| 68938-03-4 | Octene, HOF, low-boiling | | | |
| | C9 Alcohol | **10.1 mg/L** | **4.9 mg/L** | **8.5 mg/L** |
| | C8 Olefin | **0.9 mg/L** | 1.0 mg/L* | 0.7 mg/L* |
| 68526-89-6 | Octene, HOF, high-boiling | | | |
| | C9-C10 Alcohol | RA | RA | RA |
| | - | - | - | - |
| 68938-04-5 | Nonene, HOF | | | |
| | C10 Alcohol | **3.1 mg/L** | 3.0 mg/L* | 2.0 mg/L* |
| | C9 Olefin | 0.32 mg/L* | 0.41 mg/L* | 0.30 mg/L* |
| 68526-93-2 | Nonene, HOF, low-boiling | | | |
| | C10 Alcohol | **3.1 mg/L** | 3.0 mg/L* | 2.0 mg/L* |
| | C9 Olefin | 0.32 mg/L* | 0.41 mg/L* | 0.30 mg/L* |

**Table 6. Continued**

| Olefin Hydroformylation Product | | Fish Acute Toxicity 96-hour | Invertebrate Acute Toxicity 48-hour | Alga Toxicity 96-hour |
|---|---|---|---|---|
| **CAS #** | **Product Name** | | | |
| **68526-90-9** | **Nonene, HOF, high-boiling** | | | |
| | **C10-C11 Alcohol** | RA | RA | RA |
| | - | - | - | - |
| **68516-18-7** | **Decene, HOF** | | | |
| | **C11 Alcohol** | **1.8 mg/L** | 1.2 mg/L* | 0.82 mg/L* |
| | **C10 Olefin** | **0.12 mg/L** | 0.16 mg/L* | 0.12 mg/L* |
| **68527-06-0** | **Dodecene, HOF** | | | |
| | **C13 Alcohol** | **0.42 mg/L** | **0.71 mg/L** | 0.13 mg/L* |
| | **C12 Olefin** | RA | RA | RA |
| **68526-92-1** | **Dodecene, HOF, low-boiling** | | | |
| | **C13 Alcohol** | **0.42 mg/L** | **0.71 mg/L** | 0.13 mg/L* |
| | **C10-C12 Olefin** | RA | RA | RA |
| **68526-91-0** | **Dodecene, HOF, high-boiling** | | | |
| | **C13-C14 Alcohol** | RA | RA | RA |
| | - | - | - | - |

* Modeled data from ECOSAR
** Values in bold represent experimental data
RA Read Across
(†) Read across data from a C13 olefin

## Fish Acute Toxicity

Acute experimental toxicity test results are reported for rainbow trout (*Oncorhynchus mykiss*) and fathead minnow (*Pimephales promelas*)(Table 6). Experimental data for the alkyl alcohol components in olefin hydroformylation products show that they have the potential to produce an increasing level of acute toxicity to freshwater fish from approximately 98 to 0.4 mg/L for the lowest to highest molecular weight product. Experimental and modeled data for the olefin components show that they have the potential to produce an increasing level of acute toxicity in a range of 12.5 to 0.12 mg/L.

Based on chemical composition, the olefin hydroformylation products in this category are expected to produce a similar pattern of increasing acute toxicity to freshwater fish with values more closely aligned with their olefinic components. This suggests that the lowest molecular weight product (Pentene, HOF; CAS # 68527-03-7) is expected to produce a fish 96-hour toxicity value of approximately 12.5 mg/L. As the molecular weight of these products increases, acute toxicity values will decrease. The highest molecular weight product (Dodecene, HOF, high-boiling; CAS # 68526-91-0) will be the most acutely toxic with an expected fish 96-hour toxicity value of approximately 0.12 mg/L.

Experimental data for the C5, C7, and C9 olefin components are not available, but results from ECOSAR (1999), an aquatic toxicity computer model, can be used to adequately characterize the aquatic toxicity of these chemical components.

Results of computer modeling for a C6 and C8 olefin are consistent with the experimental data used to characterize the fish acute toxicity of the C6 and C8 olefin

components in this category. This suggests that the ECOSAR model is sufficiently robust to accurately calculate the toxicity of this range of chemicals. Therefore, the modeled values for a C5, C7, and C9 olefin are expected to be consistent with experimental values for these components and they will be used to characterize the range of fish acute toxicity for the olefin components of the Olefin Hydroformylation Products Category. The $K_{ow}$ values used to calculate the fish toxicity for a C5, C6, C7, C8, and C9 olefins were 2.66, 3.15, 3.64, 4.13, and 4.62, respectively. These values were calculated using the EPIWIN (1999) computer model.

**Invertebrate Acute Toxicity**

Acute experimental toxicity test results are reported for a Daphnid (*Daphnia magna*)(Table 6). Experimental and modeled data for the alkyl alcohol components in olefin hydroformylation products show that they have the potential to produce an increasing level of acute toxicity, to freshwater invertebrates, from approximately 137 to 0.7 mg/L for the lowest to highest molecular weight product. Modeled data for the olefin components show that they have the potential to produce an increasing level of acute toxicity in a range of 14.0 to 0.16 mg/L.

Based on chemical composition, the olefin hydroformylation products in this category are expected to produce a similar pattern of increasing acute toxicity to freshwater fish with values more closely aligned with their olefinic components. This suggests that the lowest molecular weight product (Pentene, HOF; CAS # 68527-03-7) is expected to produce an invertebrate 48-hour toxicity value of approximately 14.0 mg/L. As the molecular weight of these products increases, acute toxicity values will decrease. The highest molecular weight product (Dodecene, HOF, high-boiling; CAS # 68526-91-0) will be the most acutely toxic with an expected invertebrate 48-hour toxicity value of approximately 0.16 mg/L.

Experimental data for the C6 alcohol and C5, C6, C7, C8, C9, and C10 olefin components are not available, but results from ECOSAR (1999), an aquatic toxicity computer model, can be used to adequately characterize the aquatic toxicity of these components. Comparative fish acute toxicity data agree well between measured and calculated toxicity values, which suggests that this model can develop reliable toxicity data for invertebrates.

Results of computer modeling for a C7 and C8 alcohol are consistent with the experimental data used to characterize the toxicity of the C7 and C8 alcohol components in this category. As stated previously, results of computer modeling with C6 and C8 olefins are consistent when compared to experimental values for acute toxicity to fish. This suggests that the ECOSAR model is sufficiently robust to accurately calculate the toxicity of this range of chemical components, both alcohol and olefin, to freshwater invertebrates. Therefore, the modeled value for a C6 alcohol is expected to be consistent with an experimental value for a C6 alcohol in this category. Additionally, the modeled values for a C5, C6, C7, C8, C9, and C10 olefin are expected to be consistent with experimental values for the olefin components in this category. These values will be used to characterize the range of acute toxicity to invertebrates for the Olefin Hydroformylation Products Category. The $K_{ow}$ values used to calculate the

toxicity for the a C6, C7, and C8 alcohol were 1.75, 2.24, and 2.73, respectively. The $K_{ow}$ values used to calculate the toxicity for the C5 through C10 olefins were 2.66, 3.15, 3.64, 4.13, 4.62, and 5.12, respectively. These values were calculated using the EPIWIN (1999) computer model.

**Alga Toxicity**

An experimental toxicity test result is reported for the freshwater alga (*Scenendesmus quadricauda*)(Table 6) and used as read across data to the C9 alcohol component in this category). This result shows that the C9 alcohol component has the potential to cause acute toxicity (based upon cell growth) at a concentration of approximately 8.5 mg/L. However, this study is not sufficient to adequately characterize the alga toxicity of all the alcohol components in this category. Also, there are no data available for the olefin components in this category.

Although experimental data for most alcohol and all olefin components are not available, results from ECOSAR can be used to adequately characterize the aquatic toxicity of these components. Modeled data for the component chemicals (alcohol and olefin) show that these components have the potential to produce an increasing level of acute toxicity to a freshwater alga in a range of 73.2 to 0.12 mg/L. Based on chemical composition, the olefin hydroformylation products in this category are expected to produce a similar pattern of increasing acute toxicity to an alga with values more closely aligned with their olefinic components.

The ECOSAR model is sufficiently robust to accurately calculate the toxicity of this range of chemical components based on the measured and calculated values for the C9 alcohol and the comparable fish and invertebrate data (the measured alga value was 8.5 mg/L, while the calculated value was 6.0 mg/L). Therefore, the modeled values for the C6 through C13 alcohol and C5 through C12 olefin components are expected to be consistent with experimental values for their respective components in this category. These values will be used to characterize the range of acute toxicity to a freshwater alga for the Olefin Hydroformylation Products Category. The $K_{ow}$ values used to calculate the toxicity for the C6 through C13 alcohol were 1.82, 2.31, 2.81, 3.30, 3.79, 4.28, and 5.26, respectively. The $K_{ow}$ values used to calculate the toxicity for the C5 through C10 olefins were 2.66, 3.15, 3.64, 4.13, 4.62, and 5.12, respectively. These values were calculated using the EPIWIN (1999) computer model.

Experimental data for toxicity to an alga will be developed for a C6 and C13 alcohol as part of the HPV test plan for the Alkyl Alcohols C6-C13 Category (EMCCb). Experimental data for a C6 internal olefin (60-74% branched) will also be developed for the C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category (ACC, 2001). These data will be made available through the HPV Chemical Challenge Program and will be used as read across to fill the measured data gaps and to further support the expected aquatic toxicity of this category.

## E. Environmental Fate

Biodegradation data are available for three alcohol and three higher olefin components of the Olefin Hydroformylation Products Category. They show that the alcohol components of these products have the potential to biodegrade to a great extent with a standard 28-day test duration. Conversely, the olefinic components show the potential to biodegrade, but to a lesser extent within a standard 28-day test duration. These results suggest that the products in this category will not persist in the environment.

### Biodegradation

| Olefin Hydroformylation Product | | Component | | Read Across Biodegradation Strategy | Percent Biodegradation 28-days |
|---|---|---|---|---|---|
| CAS # | Product Name | Alcohol | Olefin | | |
| 68527-03-7 | Pentene, HOF | C6 | C5 | RA | RA |
| 68938-02-3 | Pentene, HOF, low-boiling | C6 | C5 | RA | RA |
| 70955-11-2 | Hexene, HOF | C7 | C6 | RA | RA |
| 70955-03-2 | Hexene, HOF, low-boiling | C7 | C6 | RA | RA |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | C6, C8 | - | RA | RA |
| 70955-04-3 | Hexene, HOF, high-boiling | C7-C8 | - | RA | RA |
| 68527-04-8 | Heptene, HOF | C8 | C7 | A, O | **82%, 29%** |
| 68526-96-5 | Heptene, HOF, low-boiling | C8 | C7 | A, O | **82%, 29%** |
| 68526-88-5 | Heptene, HOF, high-boiling | C8-C9 | - | RA | RA |
| 68527-05-9 | Octene, HOF | C9 | C8 | RA | RA |
| 68938-03-4 | Octene, HOF, low-boiling | C9 | C8 | RA | RA |
| 68526-89-6 | Octene, HOF, high-boiling | C9-C10 | - | RA | RA |
| 68938-04-5 | Nonene, HOF | C10 | C9 | A, O | **71%, 21%** |
| 68526-93-2 | Nonene, HOF, low-boiling | C10 | C9 | A, O | **71%, 21%** |
| 68526-90-9 | Nonene, HOF, high-boiling | C10-C11 | - | RA | RA |
| 68516-18-7 | Decene, HOF | C11 | C10 | RA | RA |
| 68527-06-0 | Dodecene, HOF | C13 | C12 | A | **58%** |
| 68526-92-1 | Dodecene, HOF, low-boiling | C13 | C10-C12 | A, O | **58%, 8%†** |
| 68526-91-0 | Dodecene, HOF, high-boiling | C13-C14 | - | RA | RA |

**A** **Measured data for the alcohol** (study is reliable without restriction; robust summary available).
**O** **Measured data for the olefin** (study is reliable without restriction; robust summary available).
RA Read Across (†) Read across data from a C13 olefin.

C8 and C10 alcohols have been shown to biodegrade rapidly using a 28-day standard biodegradation test procedure. In comparison, C13 alcohols biodegrade to slightly

lower but significant extent, which suggests that although they are not expected to degrade at rates equivalent to the lighter alcohol components, they will not persist in the environment. Conversely, the olefinic components show the potential to biodegrade, but to a lesser extent within a standard 28-day test duration.

Upon review of the available information, sufficient quality data were identified to accurately characterize the biodegradability of the products in this category. Based on the component data, the olefin hydroformylation products are expected to exhibit a range of biodegradation (28 days) from approximately 50 to 30% for the low to high molecular weight products, respectively. These data were developed using non acclimated inocula obtained from wastewater treatment plants. The tests used closed systems, which is recommended when assessing the biodegradability of materials with a potential to volatilize like those in this category. The test systems were continuously stirred, which is also recommended when evaluating mixtures containing several chemicals, some of which may have minimal water-solubility.

In addition, biodegradation data for a selected C5 olefin will become available from testing proposed by the American Chemistry Council, Olefins Panel in their C5 Non-Cyclics Test Plan. This data will be used to characterize the potential biodegradability of the lower molecular weight olefin hydroformylation products.

**Photodegradation – Photolysis (Direct)**

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (Zepp, 1977).

UV light absorption of the chemical components in this category will be evaluated to identify those having the potential to degrade in solution. For those compounds with a potential for direct photolysis in water, first order reaction rates will be calculated.

**Photodegradation – Atmospheric Oxidation (Indirect)**

Photodegradation can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Chemicals, such as those in the Olefin Hydroformylation Products Category, have the potential to volatilize to air.

In air, chemicals can undergo reaction with photosensitized oxygen in the form of hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based

on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for the representative chemical components in the Olefin Hydroformylation Products Category.

**Stability in Water (Hydrolysis)**

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

Stability in water can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b). However, all of the chemical structures included in the Olefin Hydroformylation Products Category are mixtures of iso-alcohols and higher olefins. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

**Chemical Transport and Distribution in the Environment (Fugacity Modeling)**

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay, 1996). EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (US EPA, 1999a), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for representative chemical components identified in products in this category. A computer model, EPIWIN – version 3.04 (EPIWIN, 1999), will be used to calculate the properties needed to run the Level I EQC model.

## IV. TEST PLAN SUMMARY

ExxonMobil Chemical believes that the olefin hydroformylation products should be further examined in the following manner:

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* for selected chemical components in this category. Provide measured data for selected products where readily available.
- Prepare a technical discussion on the potential of olefin hydroformylation products in this category to photodegrade. Calculate AOP values for selected chemical components of products in this category.
- Prepare a technical discussion on the potential of olefin hydroformylation products in this category to hydrolyze.
- Calculate fugacity data for selected chemical components of olefin hydroformylation products in this category.
- Forthcoming data on the higher olefins will be used to support read across to Olefin Hydroformylation Products for subchronic, developmental, and reproductive toxicity endpoints.

The data presented in this test plan are adequate to characterize selected HPV Program endpoints for olefin hydroformylation products. Since the olefin hydroformylation products are composed of alkyl alcohols and olefins, the available toxicity data for the alkyl alcohols and olefins are ideal for evaluating the toxicity of the olefin hydroformylation products. ExxonMobil Chemical Company believes that olefin hydroformylation products do not require further testing based on:

- Adequate toxicity data on alkyl alcohols and olefins.
- A consistent pattern of toxicity for alkyl alcohols and olefins.

ExxonMobil Chemical Company believes the thorough evaluation of the strategic anchor studies and the overall robustness of the data set for the olefin hydroformylation products category complies with the objectives of the HPV Program.

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AR201-13380B

# Olefin Hydroformylation Products Category

## Robust Summaries
## Mammalian Health Effects

| CAS Number | Product name | Olefin | Alcohol |
|---|---|---|---|
| 68527-03-7 | Pentene, HOF | C5 | C6 |
| 68938-02-3 | Pentene, HOF, low-boiling | C5 | C6 |
| 70955-11-2 | Hexene, HOF | C6 | C7 |
| 70955-03-2 | Hexene, HOF, low-boiling | C6 | C7 |
| 68526-80-7 | Alcohols, C6 and C8 iso, distillation residues | - | C6, C8 |
| 70955-04-3 | Hexene, HOF, high-boiling | - | C7-8 |
| 68527-04-8 | Heptene, HOF | C7 | C8 |
| 68526-96-5 | Heptene, HOF, low-boiling | C7 | C8 |
| 68526-88-5 | Heptene, HOF, high-boiling | - | C8-9 |
| 68527-05-9 | Octene, HOF | C8 | C9 |
| 68938-03-4 | Octene, HOF, low-boiling | C8 | C9 |
| 68526-89-6 | Octene, HOF, high-boiling | - | C9-10 |
| 68938-04-5 | Nonene, HOF | C9 | C10 |
| 68526-93-2 | Nonene, HOF, low-boiling | C9 | C10 |
| 68526-90-9 | Nonene, HOF, high-boiling | - | C10-11 |
| 68516-18-7 | Decene, HOF | C10 | C11 |
| 68527-06-0 | Dodecene, HOF | C12 | C13 |
| 68526-92-1 | Dodecene, HOF, low-boiling | C10-12 | C13 |
| 68526-91-0 | Dodecene, HOF, high-boiling | - | C13-14 |



Prepared by:

ExxonMobil Chemical Company

November 26, 2001

## Table of Contents

Developmental toxicity (1-nonanol)

C9 Hydroformylation Product ($C_9$HOF)
- Acute oral
- Acute dermal

C9 Olefin component: Alkenes, C8-10, C9 rich (68526-55-6)
- Acute oral
- Acute dermal
- Acute inhalation
- Mouse micronucleus
- Ames assay

C10 Hydroformylation Product ($C_{10}$V-HOF)
- Acute oral ($C_{10}$V-HOF)
- Acute oral ($C_{10}$U-HOF)
- Acute dermal ($C_{10}$V-HOF)
- Acute dermal ($C_{10}$U-HOF)

C10 Alcohol component: Alcohols, C9-11 iso, C10 rich (68526-85-2)
- Acute oral
- Acute dermal
- Developmental toxicity (isodecanol)
- Developmental toxicity (1-decanol)

C7-9-11 Alcohol (85566-14-9)
- Developmental toxicity

C13 Alcohol component: Alcohols, C11-14 iso, C13 rich
- Acute oral
- Ames assay (1-dodecanol)
- Repeat dose toxicity

C12 Olefin component: Alkenes, C11-13, C12 rich (68526-58-9)
- Acute oral
- Acute dermal
- Acute inhalation

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Hexanol, branched and linear |
| **CAS No.** | 68526-79-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Oral $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1960 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Males |
| **No. of animals/sex/dose** | 5 rats/dose |
| **Route of administration** | Gastric Intubation |
| **Vehicle** | None |
| **Frequency of Treatment** | Single exposure |
| **Dose/Concentration Levels** | 26, 82, 259, 820, 2591, 8200 mg/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | After a three to four hour fasting period, groups of 5 rats received the test material at dose levels of 26, 82, 259, 820, 2591, and 8200 mg/kg of body weight. The results were converted to weight units by means of the specific gravity. Observations for signs of toxicity were made immediately and at one and 24 hours after compound administration and daily for a period of 7days. Gross necropsy examinations were performed on all animals that died or were killed. |
| **Results** | $LD_{50}$= 3670 mg/kg |
| **Remarks** | None of the animals died in the 26, 82, 259, and 820 mg/kg dose groups. One of the animals in the 2591 mg/kg group died within 24 hours of dosing. All animals in the 8200 mg/kg group died within 4 hours following dose administration. Treatment resulted in depression (i.e. inactivity, depressed righting reflexes, ataxia) and labored respiration. These signs had an early onset and recovery was complete by the second day after dosing. Gross necropsy on the animals that died showed congested kidneys. Also, animals that died during the first hour after administration showed evidence of gastrointestinal irritation. |
| **Conclusions** | Under the conditions of this study, Hexanol, branched and linear has a low order of acute oral toxicity in rats. |
| **Data Quality** | 1 - Valid without restrictions |
| **Reference** | Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Hexanol, branched and linear |
| **CAS No.** | 68526-79-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute dermal toxicity |
| **GLP** | Pre-GLP |
| **Year** | 1960 |
| **Species/strain** | Albino Rabbits |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2 rabbits/sex/dose |
| **Route of administration** | Dermal Application |
| **Vehicle** | None |
| **Frequency of Treatment** | Single exposure |
| **Dose/Concentration Levels** | 82, 259, 820, and 2600 mg/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | A single dermal application of the test material was made to four groups of four rabbits at doses of 82, 259, 820, and 2600 mg/kg. The results were converted to weight units by means of the specific gravity. The test material was applied to intact abdominal skin and covered with an occlusive covering for 24 hours. Observations for signs of toxicity were made at one, four and 24 hours after compound administration and thereafter for a total of 7 days. Gross necropsies were performed on all animals at the end of the observation period. |
| **Results** | $LD_{50}$ > 2600 mg/kg |
| **Remarks** | There were no mortalities at any dosage level tested. The $LD_{50}$ in albino rabbits is greater than the highest dose tested (approx. 2.6 g/kg body weight). Signs of toxicity included labored respiration and central nervous system depression. All animals recovered within 4-48 hours after the exposure period began. Moderate erythema and edema were observed. |
| **Conclusions** | Under conditions of this study, Hexanol, branched and linear has a low order of acute dermal toxicity in rabbits. |
| **Data Quality** | 2 - Valid with restrictions. |
| **Reference** | Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Hexanol, branched and linear |
| **CAS No.** | 68526-79-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Inhalation $LC_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1960 |
| **Species/strain** | Rats/Wistar, Mice/Swiss, Guinea Pigs/English short hair |
| **Sex** | Males |
| **No. of animals/sex/dose** | 10/species |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment** | Single 6 hour exposure |
| **Dose/Concentration Levels** | 1060 ppm |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | Rats, mice, and guinea pigs received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours after exposure. |
| **Results** | $LC_{50}$ > 1060 ppm for rats, mice and guinea pigs. |
| **Remarks** | No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed in all three species. After 90 minutes of exposure, all three species exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable. |
| **Conclusions** | Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in rats, mice and guinea pigs. |
| **Data Quality** | 2 - Valid with restrictions - No analysis of exposure atmosphere. |
| **Reference** | Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report. |
| **Date last changed** | September, 2000 |

## Repeat Dose Toxicity

| | |
|---|---|
| **Test Substance** | Hexanol, branched and linear |
| **CAS No.** | 68526-79-4 |
| **Method/Guideline** | Other |
| **Test Type** | Repeated Dermal Application |
| **GLP** | Pre-GLP |
| **Year** | 1961 |
| **Species/strain** | Albino Rabbits |
| **Route of administration** | Dermal |
| **Duration of test** | 12 days |
| **Number of animals** | 8 (2/sex/dose) |
| **Dose/Conc. Levels** | 0.4 g/kg and 2.0 g/kg |
| **Sex** | Males and Females |
| **Frequency of treatment** | Single daily treatment for 10 days |
| **Control group and treatment** | Isopropyl alcohol |
| **Remarks on Test Conditions** | Undiluted control and test materials were applied to intact skin of the animals. Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each application and at study termination.<br><br>Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application and brain, liver, kidney, and blood samples were taken. In addition, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved. |
| **Results** | NOAEL for systemic toxicity = 2.0 g/kg |
| **Remarks** | There was no evidence of systemic toxicity at either dose of the test substance. Histopathological findings were unremarkable. Repeated application of the test material to the skin of albino rabbits at both dose levels produced moderate to marked degree of irritation. A slight to marked degree of edema was observed in two low-dose animals and three high-dose animals following one or more of the first three applications. Also, the exposed skin of two high-dose animals showed necrosis. |
| **Conclusions** | Under the conditions of this study, Hexanol, branched and linear can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study. |
| **Data Quality** | 2 - Valid with restrictions. |
| **Reference**: | Esso Research and Engineering Company (1961). Unpublished Report. |
| **Date last changed** | September, 2000 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | 1-Hexanol |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Not specified |
| **Year** | 1989 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Females |
| **No. of animals/sex/dose** | 15 dams/treatment |
| **Route of administration** | Inhalation |
| **Frequency of treatment** | 7 hrs/day; Gestation days 1-19 |
| **Dose/Concentration Levels** | 3500 $mg/m^3$ (Saturated vapors) |
| **Control group and treatment** | 15 sham-exposed rats |
| **Statistical methods** | MANOVA, ANOVA, Kruskal-Wallis test |
| **Remarks on Test Conditions** | Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 $mg/m^3$. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by $CO_2$ asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects. |
| **Results** | NOAEL > 3500 $mg/m^3$ |
| **Remarks** | The test substance was administered by inhalation to reflect the route of exposure found in industry. However, due to the low volatility of the alcohols, concentrations sufficient to induce maternal toxicity could not be achieved. There were no significant fetal malformations associated with inhalation of 1-hexanol by the dam. There was a slight but statistically significant increase in resorptions (1.3 vs. 0.4 per litter for controls). However, this resorption mean was still in the range seen in historical controls. |

| | |
|---|---|
| **Conclusions** | Inhalation of saturated vapors of 1-hexanol is not maternally toxic or teratogenic in rats. |
| **Data Quality** | 2 - Reliable with restrictions. |
| **Reference** | B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology evaluation of 1-pentanol, 1-hexanol, and 2-ethyl-1-hexanol administered by inhalation to rats." (1989) Journal of the American College of Toxicology **8(2)**: 405-410. NIOSH, Division of Biomedical and Behavioral Sciences |
| **Date last changed** | 13-Sep-00 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6 |
| **CAS No.** | 68526-52-3 |
| **Method** | EPA OTS 798.5395 |
| **Type of Study** | Mouse Micronucleus |
| **GLP** | Yes |
| **Year** | 1993 |
| **Species/Strain** | Mouse/ B6C3F1 |
| **Sex** | Male and Female |
| **Number/sex/dose** | 15/sex |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Exposure Period** | 6 hours/day for 2 consecutive days |
| **Concentrations** | Target exposure: 1000 ppm; Actual mean exposure: 1057 ppm (Saturated vapors, no aerosol) |
| **Controls** | Positive: Cyclophosphamide (40 mg/kg) in water by oral gavage<br>Negative: Air (Sham exposure) |
| **Statistical Methods** | To determine the percentage of micronuclei, 1000 polychromatic erythrocytes from each animal were examined for micronuclei. To determine the percentage of polychromatic erythrocytes, the number of polychromatic erythrocytes in a total of 1000 erythrocytes was determined. Statistical analysis included calculation of means and standard deviations of the micronuclei data and a test of equality of group means by a standard one way analysis of variance at each time period. When the ANOVA was significant, comparisons of carrier control to dosed group means were made according to Duncan's Multiple Range Test. Data from both males and females were analyzed as a single group to facilitate comparisons to published data. |
| **Remarks on Test Conditions** | Vapors were generated by delivering the test material with a piston pump to a glass cylinder with heating tape. Vapors were drawn into the chamber with air flow at a rate of 200 liters/minute. Nominal and actual concentrations were determined by net weight loss of the test material and by gas chromatography, respectively. Animals were exposed to vapors of the test substance for 6 hours per day on 2 consecutive days. During each exposure, animals were observed hourly. The positive control, cyclophosphamide, was administered by oral gavage as a single dose. Animals from the treated group were sacrificed by carbon dioxide asphyxiation at appropriately 24 hours after the second day of exposure. Animals treated with cyclophosphamide were sacrificed 24 hours following dose administration. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. |
| **Results** | Negative |
| **Remarks for Results** | The test material was not clastogenic since it did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, indicating that the test substance is not clastogenic. In addition, the test substance did not induce a statistically significant decrease in the mean percent of polychromatic erythrocytes, indicating that the test substance did not induce bone marrow toxicity. The positive control did induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes and was therefore clastogenic. The sham control values for the mean number of micronucleated polychromatic erythrocytes were within the normal range for the negative control. |

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|---|---|
| **Conclusions** | Under the conditions of this assay, Alkenes, C6 are not clastogenic following inhalation exposure in mice. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | "In vivo mammalian bone marrow micronucleus assay: inhalation dosing method," Exxon Biomedical Sciences, Inc. 1991 |
| **Date last changed** | December, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6 |
| **CAS No.** | 68526-52-3 |
| **Method** | EPA OTS 798.5395 |
| **Type of Study** | Mouse Micronucleus |
| **GLP** | Yes |
| **Year** | 1991 |
| **Species/Strain** | Mouse/ B6C3F1 |
| **Sex** | Male and Female |
| **Number/sex/dose** | 15/sex |
| **Route of administration** | Oral gavage |
| **Vehicle** | NA |
| **Exposure Period** | Single dose |
| **Concentrations** | 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study. |
| **Controls** | Positive: Cyclophosphamide (40 mg/kg)<br>Negative: Corn oil |
| **Statistical Methods** | To determine the percentage of micronuclei, 1000 polychromatic erythrocytes from each animal were examined for micronuclei. To determine the percentage of polychromatic erythrocytes, the number of polychromatic erythrocytes in a total of 1000 erythrocytes was determined. Statistical analysis included calculation of means and standard deviations of the micronuclei data and a test of equality of group means by a standard one way analysis of variance at each time period. When the ANOVA was significant, comparisons of carrier control to dosed group means were made according to Duncan's Multiple Range Test. A standard regression analysis was performed to test for a dose response. Sexes were analyzed separately. |
| **Remarks on Test Conditions** | The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. |
| **Results** | Positive |

| | |
|---|---|
| **Remarks for Results** | The test material induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes per 1000 cells at 5.0 g/kg for the 24-hour males and females (6.8 +/- 3.12 and 5.4 +/- 2.1, respectively). The mean number of micronucleated polychromatic erythrocytes for the positive controls at 24 hours for males and females were 36.2 +/- 10.5 and 30.4 +/- 9.0 and the negative controls were 2.4 +/- 0.9 and 2.6 +/- 1.5. The increase in micronucleated polychromatic erythrocytes observed at 24 hours was dose-related. However, at 48 and 72 hours after the initial exposure, the mean number of micronuclei did not differ between the control and treated groups. The test substance did not induce a statistically significant decrease in the mean percent of polychromatic erythrocytes, indicating that the test substance is not toxic to bone marrow. The positive control induced significant increases in the mean number of micronucleated polychromatic erythrocytes. The positive control also induced a statistically significant decrease in the mean percent of micronucleated polychromatic erythrocytes in male mice. Carrier control values for the mean percent of micronucleated polychromatic erythrocytes and the mean number of micronucleated polychromatic erythrocytes were within the normal range for the negative controls.<br><br>Alkenes, C6 produced a slight, transient increase in micronucleated polychromatic erythrocytes at the highest level by oral gavage. However, given that inhalation is the primary route of industrial exposure, a micronucleus study was repeated with inhalation as the route of administration. This study produced negative results (IUCLID section 5.6). In addition, Alkenes, C6 are not mutagenic *in vitro*. Collectively, these data suggest that Alkenes, C6 are not expected to be genotoxic. |
| **Conclusions** | Under the conditions of this study, Alkenes, C6 were clastogenic to the bone marrow of B6C3F1 mice when administered by oral gavage at 5.0 g/kg 24 hours prior to analysis, but not at 48 and 72 hours post-exposure. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | "In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method," Exxon Biomedical Sciences, Inc., 1991. |
| **Date last changed** | December, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6 |
| **CAS No.** | 68526-52-3 |
| **Method/Guideline** | EPA OTS 798.5265 |
| **Test Type** | Bacterial Mutagenicity - Ames Assay |
| **GLP** | Yes |
| **Year** | 1991 |
| **Species/strain** | Salmonella typhimurium; TA98; TA100; TA1535; TA1537; TA1538 |
| **Metabolic Activation** | With and without S9 fraction of livers from rats pretreated with Aroclor 1254. |
| **Dose/Conc. Levels** | 3.2, 10, 32, 100 and 320 μg/plate (Doses were based on a pre-test for toxicity) |
| **Statistical methods** | The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose. |
| **Remarks on Test Conditions** | |
| Solvent: | DMSO was used for controls; Ethanol was used for the test material |
| Positive Controls: | 2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine |
| Negative Controls: | Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO |
| | To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 μg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 320 μg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates. |
| | A repeat assay was performed in order to verify the data produced in the initial assay. |
| **Results** | Negative |
| **Remarks** | The test material did not induce a dose related increase in the mutation frequencies of any of the tester strains either in the presence or absence of metabolic activation. All positive and negative controls responded in a manner consistent with data from previous assays. |
| **Conclusions** | Under the conditions of this study the test material is not mutagenic for the Salmonella tester strains at doses up to and including 320 μg/plate. |
| **Data Quality** | 1 - Valid without restrictions |
| **Reference**: | Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay; Exxon Biomedical Sciences, Inc., 1991. |
| **Date last changed** | December, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C6-8 branched |
| **CAS No.** | 70914-20-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute oral toxicity |
| **GLP** | Not specified |
| **Year** | 1979 |
| **Species/strain** | Rats/Sprague/Dawley |
| **Sex** | Males |
| **No. of animals** | 5/dose |
| **Route of administration** | Oral Intubation |
| **Vehicle** | None |
| **Frequency of Treatment** | Single Exposure |
| **Dose/Concentration Levels** | 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | Animals were fasted for approximately 18 hours prior to dosing. The undiluted test material was administered by oral intubation at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg (5 rats/dose). Animals were observed for signs of toxicity at 1, 2, and 4 hours after dosing and daily thereafter for fourteen days. |
| **Results** | $LD_{50}$ = 3.9 g/kg |
| **Remarks** | All animals in the 6.81 and 10.00 g/kg groups died. Two of the five animals in the 4.64 g/kg group died and 1 animal each in the 1.00, 2.15, and 3.15 g/kg groups died. No animals in the 1.47 g/kg group died. Except for one animal in the 2.15 g/kg group, all animals that died did so within three days of dosing. Signs of toxicity observed included respiratory rate decreases, fecal staining, decreased motor activity and hypothermia. |
| **Conclusions** | Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute oral toxicity. |
| **Data Quality** | 2 - Valid with restrictions - only one sex tested. |
| **Reference** | "Acute Oral Toxicity Study in Rats," Esso Research and Engineering (1979). Unpublished report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C6-8 branched |
| **CAS No.** | 70914-20-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute dermal toxicity |
| **GLP** | Not specified |
| **Year** | 1979 |
| **Species/strain** | Albino Rabbits/New Zealand White |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2 rabbits/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | None |
| **Frequency of Treatment** | Single dose |
| **Dose/Concentration Levels** | 50, 200, 794 and 3,160 mg/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | Doses of 50, 200, 794 and 3160 mg/kg were administered to sixteen rabbits (two/sex/dose level). The undiluted test material was applied to intact skin and the animal was then wrapped in an impervious plastic sleeve. Following approximately 24 hours of exposure, the wrappings were removed and the test site was wiped free of excess test material. After 30 minutes, dermal observations were made. Observations were recorded at 1, 2 and 4 hours after dosing and daily thereafter for 14 days. |
| **Results** | $LD_{50}$ > 3,160 mg/kg of body weight. |
| **Remarks** | There were no deaths at any dose level in either sex. All animals at the 50 mg/kg level exhibited very slight erythema and no edema. Well-defined erythema without edema was observed in animals at 200 and 794 mg/kg dose levels. At the 3160 mg/kg dose level one animal exhibited moderate to severe erythema and three animals exhibited areas of necrosis. Necropsy examinations did not reveal any significant abnormalities. Dark red foci were observed in the lungs of males (50mg/kg) and females (3,160 mg/kg), however this effect was not dose-related. Dark red foci of the adrenals were observed in males and females at 200, 794, and 3,160 mg/kg. |
| **Conclusions** | Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute dermal toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions - GLP not specified. |
| **Reference** | Esso Research and Engineering (1979). Unpublished report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C6-8 branched |
| **CAS No.** | 70914-20-4 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute inhalation toxicity |
| **GLP** | Not specified |
| **Year** | 1979 |
| **Species/strain** | Rats/Sprague-Dawley, Mice/Swiss albino, Guinea pigs/Hartley |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 5/sex/dose |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment** | Single, 6 hour exposure |
| **Dose/Concentration Levels** | 0, 152 ppm |
| **Remarks on Test Conditions** | Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the total volume of air passed through the chamber to give the nominal concentration. All three species were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed. |
| **Results** | $LC_{50}$ > 152 ppm |
| **Remarks** | No abnormalities were noted in the control or exposed rats, mice or guinea pigs during the exposure period. Upon removal from the chamber, dry rales (1/10) and excessive salivation (2/10) were observed in exposed rats. During the 14-day observation period, excessive salivation was observed in mice (4/10) and nasal discharge (2/10) occurred. Necropsy examination revealed an increased incidence of lung discoloration in treated rats (6/10) and guinea pigs (8/10). |
| **Conclusions** | Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions - Vapor concentration not analyzed. |
| **Reference** | Esso Research and Engineering (1980). Unpublished Report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6-8, C7 rich |
| **CAS No.** | 68526-53-4 |
| **Method/Guideline** | NA |
| **Type of Study** | Inhalation $LC_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1979 |
| **Species/strain** | Swiss albino Mice, Sprague-Dawley Rats, Hartley Guinea Pigs |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 5/sex/species |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single Dose |
| **Dose/Concentration Levels:** | 42.3 mg/L for 6 hours; vapors only |
| **Control group and Treatment:** | Control animals (5/sex/species) were exposed to clean air as a sham exposure. |
| **Remarks on Test Conditions** | Room air, at a flow rate of 134 l/minute was bubbled through test material in a flask to produce a vapor-laden airstream that was directed, undiluted, into the exposure chamber. The nominal exposure concentration was calculated by dividing the mass of test material consumed by the total volume of air passing through the chamber.<br><br>Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. During the necropsies, the lungs with trachea, kidneys, and liver were preserved for possible histopathological examination. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LC_{50}$ > 42.3 mg/L for 6 hours** |
| **Remarks** | In mice, exposure to 42.3 mg/L of the test substance resulted in 1 death 1 hour into the exposure period. All other mice survived until the end of the study. None of the rats died during the study. Two guinea pigs died by 45 minutes into the exposure period. The remaining guinea pigs survived until the end of the study. All exposed species exhibited signs of systemic toxicity including labored breathing, prostration, body tremors, and ataxia during the exposure. However, in the surviving animals, these signs completely reversed within 24 hours following the exposure. Liver discoloration was noted upon necropsy in the mouse and the two guinea pigs that died during the exposure. Otherwise, no significant findings were observed at necropsy. |
| **Conclusions** | Under conditions of this study, Alkenes, C6-8, C7 rich have a low order of acute inhalation toxicity in rodents. |
| **Data Quality** | 2 - Valid with restrictions - no analysis of exposure atmosphere. |
| **Reference** | "An Acute Inhalation Toxicity Study of MRD-ECH-78-32 in the Mouse, Rat, and Guinea Pig," Bio/dynamics, Inc. for Exxon Research and Engineering Company, May 25, 1979. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6-8, C7 rich |
| **CAS No.** | 68526-53-4 |
| **Method/Guideline** | NA |
| **Type of Study** | Dermal $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1978 |
| **Species/strain** | Albino rabbits |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single 24-hour exposure |
| **Dose/Concentration Levels:** | 200 and 3160 mg/kg. |
| **Control group and Treatment:** | NA |
| **Remarks on Test Conditions** | Undiluted test material was applied to clipped, abraded abdominal skin under gauze and thick plastic. Following the 24-hour exposure period, the wrapping was removed and the exposed area was wiped to remove residue. Animals were observed for gross signs of irritation and systemic toxicity 1,2,3, and 4 hours post dose and daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LD_{50}$ > 3160 mg/kg** |
| **Remarks** | No mortalities were observed at any dose tested. Lethargy and ataxia were observed in all animals, but these symptoms cleared by Day 2. Dermal reactions were generally moderate at 200 mg/kg and cleared by Day 14. In the high dose group, more severe dermal reactions, including moderate edema and severe erythema, persisted through the study. No significant fluctuations in body weight occurred. Necropsy findings were unremarkable except for a pus-filled liver in 1 rabbit from the high dose group. |
| **Conclusions** | Alkenes, C6-8, C7 rich have a low order of acute dermal toxicity. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | MB Research Laboratories, Inc., Acute Dermal Toxicity in Albino Rabbits, 1978. |
| **Date last changed** | October, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C6-8, C7 rich |
| **CAS No.** | 68526-53-4 |
| **Method** | EPA OTS 798.5395 |
| **Type of Study** | Mouse Micronucleus |
| **GLP** | Yes |
| **Year** | 1993 |
| **Species/Strain** | Mouse/ B6C3F1 |
| **Sex** | Males and Females |
| **Number/sex/dose** | 15/sex |
| **Route of administration** | Oral gavage |
| **Vehicle** | NA |
| **Exposure Period** | Single dose |
| **Concentrations** | 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study. |
| **Controls** | Positive: Cyclophosphamide (40 mg/kg)<br>Negative: Corn oil |
| **Statistical Methods** | Analysis of variance (ANOVA), Duncan's Multiple Range Test |
| **Remarks on Test Conditions** | The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. |
| **Results** | Negative |
| **Remarks for Results** | There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, indicating that the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control is clastogenic. The test material did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. In addition, the test material did not induce a significant decrease in the mean percent of polychromatic erythrocytes, which is a measure of bone marrow toxicity. |
| **Conclusions** | Under the conditions of this study, the test sample is not considered to be mutagenic at doses up to and including 5.0 g/kg. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | Exxon Chemical Company (1993). In Vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Dosing Method. Unpublished Report.. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| Test Substance | Alcohols, C7-9 branched |
| CAS No. | 68526-83-0 |
| Method/Guideline | OECD 401 |
| Type of Study | Acute oral toxicity |
| GLP | Yes |
| Year | 1988 |
| Species/strain | Rats/Wistar |
| Sex | Males and Females |
| No. of animals/sex/dose | 5/sex/dose |
| Route of administration | Oral gavage |
| Vehicle | None |
| Frequency of Treatment: | Single Dose |
| Dose/Concentration Levels | 2000 mg/kg |
| Remarks on Test Conditions | After being fasted for 12 to 18 hours, animals were administered a single oral gavage dose of 2,000 mg/kg of the undiluted test article. Observations were made four times on day 1; and daily for 14 days. |
| Results | $LD_{50}$ > 2000 mg/kg |
| Remarks | Following dosing, the following symptoms were observed: sedation, ventral body position in males, hunched posture, and ruffled fur. However, all animals had recovered within 6 days of dosing. At necropsy, no macroscopic abnormalities were observed. |
| Conclusions | Under the conditions of this study, Alcohols, C7-9 branched has a low order of toxicity. |
| Data Quality | 1 – Reliable without restrictions |
| Reference | "Acute oral toxicity study with Alcohols, C7-9 branched in rats," (1988) unpublished report (RCC Research and Consulting Co. AG). |
| Date last changed | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| Test Substance | Alcohols, C7-9 branched |
| CAS No. | 68526-83-0 |
| Method/Guideline | Other |
| Type of Study | Acute dermal toxicity |
| GLP | Pre-GLP |
| Year | 1960 |
| Species/strain | Albino Rabbits |
| Sex | Males and Females |
| No. of animals/sex/dose | 4 rabbits/sex/dose |
| Route of administration | Dermal; with occlusive binding |
| Frequency of treatment | Single 24 hour exposure |
| Dose/Concentration Levels | 83, 262, 820, 2623 mg/kg (undiluted) |
| Control group and treatment | None |
| Remarks on Test Conditions | The test substance was applied dermally to rabbits (4/sex/dose) under occlusive binding and removed after 24 hours. The results were converted to weight units by means of the specific gravity. Animals were observed 1, 4, and 24 hours after initial application of Alcohols, C7-9 branched and once daily for the next 7 days. At the termination of the study, survivors were weighed and gross necropsies were performed. |
| Results | Dermal $LD_{50}$ > 2623 mg/kg |
| Remarks | Animals in the 83, 262, and 820 mg/kg dose groups exhibited normal appearance and behavior throughout the study. At the highest dose (2623 mg/kg), animals exhibited labored respiration and were inactive. One animal in the high dose group died within 24 hours. The remaining animals in this dose group returned to normal appearance and behavior 2 days after the treatment. |
| Conclusions | Alcohols, C7-9 branched showed a low order of acute dermal toxicity under the conditions of this study. |
| Data Quality | 1 - Reliable without restrictions |
| Reference | Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report. |
| Date last changed | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| Test Substance | Alcohols, C7-9 branched |
| CAS No. | 68526-83-0 |
| Method/Guideline | Other |
| Type of Study | Acute inhalation toxicity |
| GLP | Pre-GLP |
| Year | 1960 |
| Species/strain | Rats/Wistar, Mice/Swiss, Guinea pigs/English Short Hair |
| Sex | Males |
| No. of animals/sex/dose | 10/species |
| Route of administration | Inhalation |
| Vehicle | NA |
| Frequency of Treatment: | Single 6 hour exposure |
| Dose/Concentration Levels | Saturated Vapors |
| Remarks on Test Conditions | Rats, mice, and guinea pigs were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed. |
| Results | $LC_{50}$ > 200 ppm |
| Remarks | There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior other than blinking in rats and mice. No macroscopic abnormalities were observed at necropsy. |
| Conclusions | Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in rats, mice and guinea pigs. |
| Data Quality | 2 - Valid with restrictions. No analysis of exposure atmosphere. |
| Reference | Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report. |
| Date last changed | September, 2000 |

## Genetic Toxicity

| | |
|---|---|
| Test Substance | 2-Ethyl-1-hexanol |
| CAS No. | 104-76-7 |
| Method | Other |
| Type of Study | Ames Assay |
| Test System | *S. typhimurium, E. coli* |
| GLP | Not specified |
| Year | 1985 |
| Species/Strain | *Salmonella typhimurium* /TA98; TA100; TA1535; TA1537; TA1538; *E. coli* WP2uvrA |
| Metabolic Activation | S9 mixture |
| Concentrations | 1, 5, 10, 50, 100, 500, and 1000 ug/plate. |
| Statistical methods | Samples were run in duplicate. No further details provided. |
| Remarks on Test Conditions | 2-Ethyl-1-hexanol (98% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (Polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)-acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls. |
| Results | Negative |
| Remarks for Results | In all of the strains tested, there was no evidence of mutagenicity of 2-ethyl-1-hexanol in the presence or absence of metabolic activation. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 2-ethyl-1-hexanol samples. |
| Conclusions | 2-Ethyl-1-hexanol is not mutagenic in bacteria under the conditions of this study. |
| Data Quality | 2- Reliable with restrictions (Similar to OECD 471) |
| Reference | H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," *Japanese Journal of Industrial Health*, 27: 400-419. |
| Date last changed | October 3, 2000 |

## Repeat Dose Toxicity

| | |
|---|---|
| Test Substance | Iso-octanol |
| CAS No. | -- |
| Method/Guideline | NA |
| Type of Study | 14-day repeat dose |
| GLP | Not specified |
| Year | 1984 |
| Species/strain | Rats/Wistar |
| Sex | Male |
| No. of animals/sex/dose | 5/treatment, 10/control; 1mmol/kg/day of iso-octanol (130 mg/kg/day) |
| Route of administration | Oral gavage. |
| Duration of test | 14 days |
| Frequency of treatment | Once daily for 14 days |
| Vehicle | Polyethylene glycol 300 |
| Statistics | Mean values compared to controls by Student's t-test. |
| Remarks on Test Conditions | After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined. |
| Results | NOAEL = 130 mg/kg/day |
| Remarks | Iso-octanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Iso-octanol did not induce any changes in glycogen vacuolation or fat vacuolation. The activity of peroxisome-associated enzymes and levels of cholesterol and triglyceride were not significantly different between animals treated with iso-octanol and vehicle controls. No hyperlipidemia was observed. |
| Conclusions | Under the conditions of this study, iso-octanol had a low order of sub-acute toxicity in male rats for the endpoints studied. |
| Data Quality | 2 - Reliable with restrictions - Not a guideline study. |
| Reference | C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). Toxicology Letters 21: 103-109. |
| Date last changed | 13-Sep-00 |

## Repeat Dose Toxicity

| | |
|---|---|
| Test Substance | Alcohols, C7-9 branched |
| CAS No. | 68526-83-0 |
| Method/Guideline | Other |
| Test Type | Repeated Dermal Application |
| GLP | Pre-GLP |
| Year | 1961 |
| Species/strain | Albino Rabbits |
| Route of administration | Dermal |
| Duration of test | 12 days |
| Number of animals | 8 rabbits (2/sex/dose) |
| Dose/Conc. Levels | 0.4 g/kg and 2.0 g/kg |
| Sex | Males and Females |
| Frequency of treatment | Single Daily treatment for 10 days |
| Control group | Isopropyl alcohol, 2/sex |
| Statistical methods | Not specified |
| Remarks on Test Conditions | Undiluted control and test materials were applied to intact skin of the animals (2/sex/dose). Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each exposure and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved. |
| Results | NOAEL for systemic toxicity = 2.0 g/kg |
| Remarks | Animals in all exposure groups displayed normal appearance and behavior throughout the study. Although a slight decrease in body weight was observed initially, animals regained weight by the end of the study. Repeat application of the control substance, isopropyl alcohol produced slight irritation characterized by slight to moderate erythema, atonia, and desquamation. Repeated application of Alcohols, C7-9 branched resulted in moderate to severe irritation. Fissuring and coriaceous skin were also observed at both the low and high dose levels. Necrosis was observed in the high dose animals as well. Clinical studies did not indicate any other signs of toxicity. There was a general increase in the hematocrit and erythrocyte values at the end of the study. |

| | |
|---|---|
| Conclusions | Under the conditions of this study, Alcohols, C7-9 branched can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study. |
| Data Quality | 2 - Valid with restrictions |
| Reference | Esso Research and Engineering Company (1961). Repeat Dermal Application of Alcohols, C7-9 branched, Unpublished Report. |
| Date last changed | September, 2000 |

## Developmental Toxicity

| | |
|---|---|
| Test Substance | 1-Octanol |
| CAS No. | NR |
| Method/Guideline | Other |
| Type of Study | Developmental Toxicity |
| GLP | Not specified |
| Year | 1989 |
| Species/strain | Rats/Sprague-Dawley |
| Sex | Pregnant females |
| No. of animals/sex/dose | 15/dose |
| Route of administration | Inhalation |
| Frequency of treatment | 7 hrs/day; Gestation days 1-19 |
| Dose/Concentration Levels | 400 $mg/m^3$ |
| Control group and treatment | 15 sham-exposed rats |
| Statistical methods | MANOVA, ANOVA, Kruskal-Wallis test |
| Remarks on Test Conditions | Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 400 $mg/m^3$. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by $CO_2$ asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects. |
| Results | Maternal and Developmental NOAEL ≥ 400 $mg/m^3$ |

| | |
|---|---|
| Remarks | No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups. |
| Conclusions | Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Octanol does not induce maternal or fetal toxicity. |
| Data Quality | 2 - Reliable with restrictions |
| Reference | B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology 9(1): 93-97. NIOSH, Division of Biomedical and Behavioral Sciences. |
| Date last changed | February, 2001 |

## Developmental Toxicity

| | |
|---|---|
| Test Substance | Alcohols, C7-9 branched |
| CAS No. | 68526-83-0 |
| Method/Guideline | OECD 414 |
| Type of Study | Developmental Toxicity |
| GLP | Yes |
| Year | 1994 |
| Species/strain | Rat/Sprague-Dawley |
| Sex | Females |
| No. of animals/dose | 25/dose |
| Route of administration | Oral gavage |
| Exposure period | GD 6-15 |
| Dose/Concentration Levels | 100, 500, and 1000 mg/kg/day |
| Control group and treatment | Carrier only - corn oil |
| Statistical methods | Nested analysis of covariance, Least Significant Difference (LSD), Chi-square, Fisher Exact test, Armitage's test. |
| Remarks on Test Conditions | Mated females were assigned to dose groups of 100, 500, and 1000 mg/kg/day or to a corn oil-only group (25/dose). The test substance was administered in volumes of 5 ml/kg. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. The animals were examined for viability twice daily during the treatment period and once daily thereafter. Clinical observations were made daily during gestation. On GD 21, animals were sacrificed and cesarean sections and necropsies were performed. Uterine weights with ovaries attached were recorded, uterine contents were examined, and implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations. Approximately one-half of the fetuses were prepared for examination of abnormalities in the head and the other half were preserved for examination of skeletal abnormalities. |
| Results | Maternal NOAEL = 500 mg/kg/day<br>Fetal NOAEL = 1000 mg/kg/day |
| Remarks | One animal in the high dose group was euthanized in moribund condition on GD 9. The animal had extreme abdominal staining just prior to death, but there were no significant findings at postmortem examination and the cause of morbidity was therefore not established. Adverse clinical signs were observed in 8 of the 24 dams in the high dose group. These signs included emaciation, decreased food consumption, abdominal/anogenital staining, rales, hypoactivity, and little or no stool. The symptoms were transient and generally were not observed following cessation of dosing. The remaining dams in the high dose group had incidental findings such as alopecia, but otherwise appeared normal throughout the study. There were no observable abnormalities in dams of the middle and low dose groups throughout the gestational period. In the high dose group, statistically significant decreased body weight gain and food consumption were observed from GD 6-9 and GD6-15 compared to controls. However, these effects subsided after cessation of treatment and body weight and food consumption for the overall gestational period (GD 6-21) were not significantly different between the high dose group and controls. There were no maternal findings at necropsy that were judged to be the result of treatment with Alcohols, C7-9 branched. For the most part, uterine implantation parameters were equivalent between the treated and control groups. |

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|---|---|
| Remarks, cont'd | There were slight differences between the high dose group and the control group in the number of post-implantation losses and resorptions, however these differences were not statistically significant and were deemed to be due to the poor health of the dams.<br><br>Mean fetal body weight was equivalent between treated and control fetuses of both sexes. Three low dose, two mid dose, and one high dose fetus were stunted. There were no statistically significant differences in mean skeletal ossification sites and in total or individual external, visceral, or skeletal malformations between control and treated groups. There were statistically significant increases in total fetuses with skeletal variations and in the incidence of hypoplastic skull bones in the high dose group when compared to controls. These findings were slightly higher than the historical control range of the lab and were not observed with litter-based analysis. Statistically significant increases in the number of lumbar ribs were observed in the middle and high dose groups. However, due to the lack of embryotoxicity observed in this study, these findings were attributed to maternal toxicity observed during treatment. |
| Conclusions | Under the conditions of this study, Alcohols, C7-9 branched induces maternal toxicity at concentrations that are not embryotoxic. |
| Data Quality | 1 - Reliable without restrictions |
| Reference | Exxon Biomedical Sciences, Inc. (1994). Developmental Toxicity Study in Rats, Unpublished report. |
| Date last changed | February, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C7-9, C8 rich |
| **CAS No.** | 68526-54-5 |
| **Method/Guideline** | NA |
| **Type of Study** | Oral $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1975 |
| **Species/strain** | Albino Rats |
| **Sex** | Male |
| **No. of animals/sex/dose** | 10 rats |
| **Route of administration** | Oral gavage |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single Treatment |
| **Dose/Concentration Levels:** | 5000 mg/kg |
| **Control group and Treatment:** | NA |
| **Remarks on Test Conditions** | A single dose of undiluted test material (5,000 mg/kg) was administered to male rats (not fasted). Individual body weights were recorded on Day 0 and Day 7. Gross necropsy examinations were performed on all animals that died or were killed. |
| **Results ($LD_{50}$ or $LC_{50}$):** | $LD_{50}$ > 5000 mg/kg |
| **Remarks** | Hypoactivity and diarrhea were noted within 6-22 hours post-oral administration and subsided by the second post-oral exposure day. There were no significant findings observed during the gross necropsy examination. |
| **Conclusions** | Under the conditions of this study, Alkenes, C7-9, C8 rich have a low order of acute oral toxicity. |
| **Data Quality** | 1 - Reliable without restrictions, comparable to a guideline study |
| **Reference** | Exxon Research and Engineering Company (1975). Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study. Unpublished Report. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C7-9, C8 rich |
| **CAS No.** | 68526-54-5 |
| **Method/Guideline** | NA |
| **Type of Study** | Dermal $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1975 |
| **Species/strain** | Albino rabbits |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single 24-hour exposure |
| **Dose/Concentration Levels:** | 200, 3160 mg/kg. |
| **Control group and Treatment:** | NA |
| **Remarks on Test Conditions** | A single dermal application of the test material was made to four groups of four rabbits at doses of 200 and 3,160 mg/kg. The test material was applied to abraded skin. Individual body weights were recorded on Days 0, 7 and 14. Gross necropsies were performed at the end of the experiment. |
| **Results ($LD_{50}$ or $LC_{50}$):** | $LD_{50}$ > 3,160 mg/kg |
| **Remarks** | There were no mortalities at any dosage level tested. Thus, the $LD_{50}$ in albino rabbits is greater than the highest dose tested. Signs of erythema, mild to moderate edema and second degree burns were observed at 24 hours at both doses. At 7 and 14 days, focal escharosis was observed at the low dose. At the high dose, escharosis, fissuring, hemorrhaging, and wrinkling were observed at 7 days and escharosis was observed at 14 days. Necropsy examination revealed emaciation and depletion of fat stores in one male rabbit in the low dose group. No other gross pathologic alterations were observed. |
| **Conclusions** | Alkenes, C8-10, C9 rich have a low order of acute dermal toxicity. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | Exxon Research and Engineering Company (1975). Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study. Unpublished Report. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

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|---|---|
| **Test Substance** | Alkenes, C7-9, C8 rich |
| **CAS No.** | 68526-54-5 |
| **Method/Guideline** | NA |
| **Type of Study** | Inhalation $LC_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1977 |
| **Species/strain** | Albino rats, mice, and guinea pigs |
| **Sex** | Males |
| **No. of animals/sex/dose** | 10/species |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single 6-hour Exposure |
| **Dose/Concentration Levels:** | 31.67 mg/L |
| **Control group and Treatment:** | Control animals were exposed to clean air at the same flow rate as the treated group. |
| **Remarks on Test Conditions** | Rats, mice, and guinea pigs received a single, 6-hour exposure to the test material. The exposure was conducted in a 1000-liter glass and stainless steel chamber. The compound was placed in a 2000 ml three-necked flask, pre-weighed and mounted outside the chamber. Air was bubbled through the test material at 5 L/min and was then combined with an additional airflow of 10 L/min to produce a total flow rate through the chamber of 15 L/min.<br><br>All animals were observed for signs of toxicity, abnormal behavior, and mortality during the exposure period and for 14 days after the exposure. Necropsies were performed on all surviving animals and any animals that died during the exposure or post-exposure observation period. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LC_{50}$ > 31.7 mg/L (rat)**<br>**$LC_{50}$ > 31.7 mg/L (mouse)**<br>**$LC_{50}$ < 31.7 mg/L (guinea pig)** |
| **Remarks** | There were no deaths in the air-exposed animals. In the treated animals, six guinea pigs and three rats died during the exposure period. No mice died during the study. One guinea pig died on Day 1 of the recovery period. All animals showed compound awareness 1 minute after exposure began and became increasingly agitated during the first 35 minutes of exposure. After 100 minutes, some animals were experiencing tremors and convulsions. Necropsy examination indicated dark red coloration of the lungs of 15 animals (3 rats, 4 mice, and 8 guinea pigs). Six guinea pigs had liver discolorations. Five guinea pigs showed pale kidney color also. One guinea pig that died showed a large amount of blood in the heart. Fifteen animals (7 rats, 6 mice, and 2 guinea pigs) showed no gross lesions. |
| **Conclusions** | Under conditions of this study, Alkenes, C7-9, C8 rich have a low order of acute inhalation toxicity in rats. |
| **Data Quality** | 1 - Valid without restrictions; Comparable to a guideline study. |
| **Reference** | Exxon Corporation (1977). Acute Inhalation Toxicity- Rats, mice and guinea pigs. Unpublished Report. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

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|---|---|
| **Test Substance** | Alcohols, C8-10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline** | NA |
| **Type of Study** | Acute oral toxicity |
| **GLP** | Pre-GLP |
| **Year** | 1968 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Males |
| **No. of animals/sex/dose** | 5/dose |
| **Route of administration** | Gastric Intubation |
| **Vehicle** | None |
| **Frequency of Treatment** | Single Exposure |
| **Dose/Concentration Levels** | 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | After a three to four hour fasting period, groups of 5 rats (approximately 252-295 grams) received the undiluted test material at doses of 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg body weight. Observations were recorded immediately after dosing; at one, four and 24 hours; and once daily for a total of 14 days. |
| **Results** | $LD_{50}$ = 2979 mg/kg |
| **Remarks** | No deaths occurred in the 34.6, 120, 417, and 1450 mg/kg groups throughout the study. Two of the five animals in the 5000 mg/kg group died within 24 hours and all of the animals in the 10,000 mg/kg group died within 24 hours. Depression, labored respiration and evidence of excessive urination and/or diarrhea were observed at the 5,000 and 10,000 mg/kg dose levels. These signs of toxicity were observed within one hour of administration. At necropsy, abscessed lungs, dark red lungs and a dark zone between the renal cortex and medulla were observed in animals from the 5,000 and 10,000 mg/kg dose levels. |
| **Conclusions** | Under conditions of this study, Alcohols, C8-10 iso, C9 rich have a low order of acute oral toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions (Pre-GLP) |
| **Reference** | Esso Research and Engineering (1968). Unpublished report. |
| **Date last changed** | September, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C8-10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute dermal toxicity |
| **GLP** | Pre-GLP |
| **Year** | 1968 |
| **Species/strain** | Rabbits/New Zealand White |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2/sex/dose |
| **Route of administration** | Dermal |
| **Frequency of Treatment** | Single Exposure |
| **Dose/Concentration Levels** | 50, 200, 794 and 3,160 mg/kg |
| **Remarks on Test Conditions** | A single application of the test material was made to four groups of four rabbits (2.0 to 2.8 kg) at doses of 50, 200, 794 and 3160 mg/kg. The material was applied to abraded abdominal skin under occlusive dressing. Observations were recorded immediately following application; at one, four and 24 hours; and once daily thereafter for a total of 14 days. |
| **Results** | $LD_{50}$ > 3,160 mg/kg of body weight. |
| **Remarks** | No deaths were observed at any timepoint in this study. No evidence of systemic toxicity was observed. Dose-related moderate to severe skin irritation was produced. For all of the doses tested, no compound-related alterations were observed at necropsy. |
| **Conclusions** | Under the conditions of this study, Alcohols, C8-10 iso, C9 rich has a low order of acute dermal toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions (Pre-GLP) |
| **Reference** | Esso Research and Engineering (1968). Unpublished report. |
| **Date last changed** | September, 2000 |

## Repeat Dose Toxicity

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|---|---|
| **Test Substance** | Isononanol |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | 14-day repeated dose |
| **GLP** | Not specified |
| **Year** | 1983 |
| **Species/strain** | Rats /Wistar |
| **Sex** | Male |
| **No. of animals/sex/dose** | 5/treatment, 10/control; 1mmol/kg/day of isononanol (144 mg/kg/day) |
| **Route of administration** | Oral gavage. |
| **Frequency of treatment** | Once daily for 14 days |
| **Vehicle** | Polyethylene glycol 300 |
| **Statistical methods** | Mean values compared to controls by Student's t-test. |
| **Remarks on Test Conditions** | After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined. |
| **Results** | NOAEL ≥ 144 mg/kg/day |
| **Remarks** | Isononanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Isononanol did not induce any changes in glycogen vacuolation or fat vacuolation. The levels of cholesterol and triglyceride were not significantly different between animals treated with isononanol and vehicle controls. There was a slight induction of palmitoyl CoA oxidase activity. However, the activity of other peroxisome-associated enzymes was not affected and overall peroxisome number was not effected. No hyperlipidemia was observed. |
| **Conclusions** | Under the conditions of this study, isononanol has a low order of sub-acute toxicity in male rats for the endpoints studied. |
| **Data Quality** | 2 - Valid with restrictions. Not a guideline study. |
| **Reference** | C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). Toxicology Letters **21**: 103-109. |
| **Date last changed** | 13-Sep-00 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | Isononylalcohol 1 |
| **CAS No.** | 68515-81-1 |
| **Method/Guideline** | OECD 414 |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Yes |
| **Year** | 1989 |
| **Species/strain** | Rats/Wistar |
| **Sex** | Females |
| **No. of animals/sex/dose** | 10/dose |
| **Route of administration** | Oral gavage |
| **Vehicle** | Aqueous emulsion in 0.005% Cremophor EL |
| **Frequency of Treatment** | Gestation days 6-15 |
| **Dose/Concentration Levels** | 144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) |
| **Control group and Treatment** | Control Group 1: Doubly distilled water<br>Control Group 2: Doubly distilled water with 0.005% Cremophor EL |
| **Statistical Methods** | Dunnett's test, Fisher's exact test |
| **Remarks on Test Conditions** | The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings. |
| **Results** | NOAEL = 144 mg/kg/day (Maternal and Fetal) |
| **Remarks** | At the lowest dose level, no maternal toxicity was observed. There were an increased number of fetuses with hydroureter. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. At both the 144 and 720 mg/kg/day dose levels, there were no effects on the following parameters: uterine weight, conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, and viable fetuses. At the 720 mg/kg/day level, the following signs of maternal toxicity were observed - reduced food consumption, reduced body weight, unsteady gait, and reddish nasal discharge. Fetal effects included a slightly reduced mean fetal body weight and an increased number of fetuses with hydroureter. Signs of maternal toxicity at the 1440 mg/kg/day level included reduced rood consumption and mean body weight, severe clinical symptoms like abdominal or lateral position, and unsteady gait. In addition, 7 of the animals found dead by gestation day 11 and the remaining 3 were sacrificed in moribund condition by gestation day 10. At necropsy, all animals had light brown-gray discoloration of the liver and some had evidence of lung edema and petechiae in the lungs. Because of the death of all dams within the high dose group, no data were available to assess uterus weight, reproduction parameters, or fetal effects. |

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| **Conclusions** | When administered by oral gavage under the conditions of this study, Isononylalcohol 1 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononylalcohol 1 does not alter reproductive parameters at doses that are not maternally toxic. |
| **Data Quality** | 2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed. |
| **Reference** | Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247. |
| **Date last changed** | February, 2001 |

## Developmental Toxicity

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|---|---|
| **Test Substance** | Isononylalcohol 2 |
| **CAS No.** | 68515-81-1 |
| **Method/Guideline** | OECD 414 |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Yes |
| **Year** | 1989 |
| **Species/strain** | Rats/Wistar |
| **Sex** | Females |
| **No. of animals** | 10/group |
| **Route of administration** | Oral gavage |
| **Frequency of Treatment** | Gestation days 6-15 |
| **Dose/Concentration Levels** | 144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) |
| **Control Group and Treatment** | Control Group 1: Doubly distilled water<br>Control Group 2: Doubly distilled water with 0.005% Cremophor EL |
| **Statistical methods** | Dunnett's test, Fisher's exact test |
| **Remarks on Test Conditions** | The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings. |
| **Results** | NOAEL = 144 mg/kg/day |
| **Remarks** | At the lowest dose level, no maternal or fetal toxicity was observed. In addition, there were no changes in reproductive parameters. At the 720 mg/kg/day level, signs of maternal toxicity included unsteady gait, piloerection, salivation, and reduced body weight gain and food consumption. There was also an increased frequency of fetuses with hydroureter at this level. At this level, there were no significant changes in reproductive parameters. Although there was an increased number of late resorptions, this number was within the range of biologic variation, was not dose-dependent, and was therefore considered incidental.<br><br>At the highest dose level, dams exhibited marked decreases in weight gain and food consumption, and displayed severe clinical symptoms, including unsteady gait, apathy, and abdominal or lateral position. One animal was found dead on gestation day 9 and two other dams were sacrificed in moribund condition on gestation days 8 and 109. At necropsy, light brown-gray discoloration of the liver, lung edema, and petechiae in the lungs, heart, or bladder were observed. Fetuses from the high dose group had markedly reduced mean fetal body weight, increased frequency of hydroureter, and a higher frequency of fetuses with skeletal variations and retardations. At the highest dose, there were no changes in fertility parameters. |

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|---|---|
| **Conclusions** | When administered by oral gavage under the conditions of this study, Isononylalcohol 2 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononyl alcohol 2 does not alter fertility parameters at doses that are not maternally toxic. |
| **Data Quality** | 2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed. |
| **Reference** | Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247. |
| **Date last changed** | February, 2001 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | 1-Nonanol |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Not specified |
| **Year** | 1989 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Pregnant females |
| **No. of animals/sex/dose** | 15 dams/dose |
| **Route of administration** | Inhalation |
| **Frequency of treatment** | 7 hrs/day; Gestation days 1-19 |
| **Dose/Concentration Levels** | 150 mg/m$^3$ (Saturated vapors) |
| **Control group and treatment** | 15 sham-exposed rats |
| **Statistical methods** | MANOVA, ANOVA, Kruskal-Wallis test |
| **Remarks on Test Conditions** | Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m$^3$. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by $CO_2$ asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects. |
| **Results** | NOAEL = 150 mg/m$^3$ |
| **Remarks** | No treatment-related effects were observed in dams. There were no statistically significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. There were no statistically significant differences between the mean number of corpora lutea and resorptions, the sex ratio, and the mean fetal weights between the control and treated groups. |

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| **Conclusions** | Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Nonanol does not induce maternal or fetal toxicity. |
| **Data Quality** | 2 - Reliable with restrictions - Similar to guideline study; only one exposure level. |
| **Reference** | B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology **9(1)**: 93-97. NIOSH, Division of biomedical and behavioral sciences |
| **Date last changed** | February, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_9HOF$ |
| **CAS No.** | |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Oral |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rats |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 5/sex/dose |
| **Route of administration** | Oral |
| **Vehicle** | NA |
| **Dose/Concentration Levels** | 5000 mg/kg |
| **Remarks on Test Conditions** | Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose. Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel. |
| **Results** | $LD_{50}$ > 5000 mg/kg |
| **Remarks** | All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area in some animals. Nine of the ten animals exhibited no observable abnormalities through the second week of the study. Upon postmortem examination, slightly discolored lungs, maloccluded incisors, slight alopiecia, and red staining around the eye were observed in two of the animals. Eight of the ten test animals exhibited no observable abnormalities at necropsy. |
| **Conclusions** | Under the conditions of this study, $C_9HOF$ has a low order of acute oral toxicity. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | "Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_9HOF$ |
| **CAS No.** | |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Dermal |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rabbit |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 3/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Dose/Concentration Levels** | 3160 mg/kg |
| **Remarks on Test Conditions** | Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The test material was covered with a gauze patch and secured with tape. To prevent evaporation or ingestion of the test material, the gauze patch was secured to the trunk of the animal with tape and a plastic sleeve. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed. |
| **Results** | $LD_{50}$ > 3160 mg/kg |
| **Remarks** | There were no deaths prior to study termination. At study termination, all animals displayed an increase in body weight over their initial body weights. Clinical in-life observations were minimal and included nasal discharge, abdominal staining, staining in the anogenital area, thin hair coat, soft stool, and alopecia. Gross necropsy revealed single incidences of anogenital staining, thin hair coat, and alopecia. Three of the six test animals exhibited no observable abnormalities. Dermal observations included well-defined to moderate-to-severe erythema and slight edema at 72 hours. However, irritation decreased by Day 14 and only slight erythema and edema were observed in one animal by Day 14. The remaining animals showed no signs of irritation by Day 14. |
| **Conclusions** | Under the conditions of this study, $C_9HOF$ has a low order of acute toxicity by the dermal route of exposure. |
| **Data Quality** | 1 - Reliable without restrictions. |
| **Reference** | "Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C8-10, C9 rich |
| **CAS No.** | 68526-55-6 |
| **Method/Guideline** | NA |
| **Type of Study** | Oral $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1957 |
| **Species/strain** | Rats/Holtzman |
| **Sex** | Male |
| **No. of animals/sex/dose** | 5/dose |
| **Route of administration** | Oral gavage |
| **Vehicle** | 0.5% aqueous methyl cellulose solution |
| **Frequency of Treatment:** | Single Treatment |
| **Dose/Concentration Levels:** | 0.1, 1.0, and 10.0% volume/volume in a 0.5% aqueous methyl cellulose solution. (Equivalent to 7.4, 23.3, 73.8, 233, 738, 2332 mg/kg) |
| **Control group and Treatment:** | For comparison, untreated animals were necropsied at the end of the study. |
| **Remarks on Test Conditions** | Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water were available at all times. The animals were observed for gross effects and mortality several times on the day of exposure and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period. |
| **Results ($LD_{50}$ or $LC_{50}$):** | $LD_{50}$ > 2332 mg/kg |
| **Remarks** | No mortalities were observed at any of the doses tested. Animals in the high dose group appeared slightly depressed the day after administration of the test material. For several hours following exposure, the animals in the high dose group also showed slight nasal discharge. Otherwise, all animals appeared normal throughout the study. Animals in all groups exhibited normal weight gain. Gross necropsy did not reveal any abnormalities other than slightly congested adrenal glands in animals from the three higher dose levels (233, 738, and 2332 mgl/kg). |
| **Conclusions** | Under the conditions of this study, Alkenes, C8-10, C9 rich have a low order of toxicity. |
| **Data Quality** | 2 - Reliable with restrictions, comparable to a guideline study (pre-GLP). |
| **Reference** | Hazleton Laboratories for Esso Research and Engineering Co., Acute Oral Administration, 1957. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C8-10, C9 rich |
| **CAS No.** | 68526-55-6 |
| **Method/Guideline** | NA |
| **Type of Study** | Dermal $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1957 |
| **Species/strain** | Albino rabbits |
| **Sex** | Males |
| **No. of animals/sex/dose** | 4/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single 24-hour exposure |
| **Dose/Concentration Levels:** | 73.8, 233, 738, 2332 mg/kg. |
| **Control group and Treatment:** | NA |
| **Remarks on Test Conditions** | Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LD_{50}$ > 2332 mg/kg** |
| **Remarks** | No mortalities were observed at any dose tested. The abdomens and binders were dry at the end of the exposure period, indicating a good rate of dermal absorption of the applied material. The test material produced mild dermal irritation characterized by mild erythema. Most of the animals showed slight atonia for several days of the observation period and desquamation during the final two days of the observation period. Throughout the study, all animals exhibited normal appearance and behavior. Body weight gain was normal throughout the study. There were no significant findings at necropsy. |
| **Conclusions** | Alkenes, C8-10, C9 rich have a low order of acute dermal toxicity. |
| **Data Quality** | 2 - Reliable with restrictions. Pre-GLP. |
| **Reference** | Hazleton Laboratories for Esso Research and Engineering Co., Acute Dermal Application, 1957. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C8-10, C9 rich |
| **CAS No.** | 68526-55-6 |
| **Method/Guideline** | Other |
| **Type of Study** | Inhalation $LC_{50}$ |
| **GLP** | Not specified |
| **Year** | 1977 |
| **Species/strain** | CD-1 Mice, Sprague-Dawley Rats, Hartley Guinea Pigs |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 5/sex/species |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single Dose |
| **Dose/Concentration Levels:** | 11.1 mg/L for 6 hours |
| **Control group and Treatment:** | Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group. |
| **Remarks on Test Conditions** | An airstream was bubbled through the test material at a rate of 33.1 L/min and passed through a 760 L test chamber containing the test animals for a total of 6 hours. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LC_{50}$ > 11.1 mg/L for 6 hours** |
| **Remarks** | None of the animals died during the exposure period or during the 14-day post-exposure observation period. A total of 132.1 g of test material was delivered to the chamber during the course of the exposure. The overall nominal concentration of the test substance was 11.1 mg/L. During the last 4 hours of exposure, mice exhibited labored breathing patterns, rats exhibited limb ataxia and generally lethargic behavior, and the guinea pigs showed slight tremors. No similar signs were noted in the control animals, indicating that these effects were due to exposure to the test substance. However, all of the symptoms subsided as the test chamber was cleared with clean air. On day 4 of the post-exposure observation period, one of the exposed mice had tremors, but the symptoms only occurred on that day and were not believed to be due to exposure to the test substance. Signs of toxicity observed during the 14-day post-exposure period included dry rales, soft stool, and nasal discharge in rats, however, these signs were observed in both the exposed and control animals and are not believed to be due to the test substance. In both exposed animals and controls, there was a slight decrease in body weight during the first few days following exposure, after which the animals recovered their normal body weight. There were no significant differences observed between the exposed animals and the test animals at necropsy. Although there was a high incidence of kidney lesions in both groups of guinea pigs, the rate was slightly higher in the exposed animals than in the controls. However, the difference was not statistically significant. |
| **Conclusions** | Under conditions of this study, Alkenes, C8-10, C9 rich have a low order of acute inhalation toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions. No analysis of exposure atmosphere. |
| **Reference** | "An Acute Inhalation Toxicity Study of MRD-76-57 in the Mouse, Rat, and Guinea Pig," Bio/dynamics, Inc. for Exxon Research and Engineering Company, April 11, 1977. |
| **Date last changed** | October, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C8-10, C9 rich |
| **CAS No.** | 68526-55-6 |
| **Method** | EPA OTS 798.5395 |
| **Type of Study** | Mouse Micronucleus |
| **GLP** | Yes |
| **Year** | 1991 |
| **Species/Strain** | Mouse/ B6C3F1 |
| **Sex** | Male and Female |
| **Number/sex/dose** | 15/sex |
| **Route of administration** | Oral gavage |
| **Vehicle** | NA |
| **Exposure Period** | Single dose |
| **Concentrations** | 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study. |
| **Controls** | Positive: Cyclophosphamide (40 mg/kg)<br>Negative: Corn oil |
| **Statistical Methods** | Analysis of variance (ANOVA), Duncan's Multiple Range Test |
| **Remarks on Test Conditions** | The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. |
| **Results** | Negative |
| **Remarks for Results** | There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. Thus, the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control is clastogenic. The test material did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. However, the test material did induce a significant decrease in polychromatic erythrocytes in both males and females at 48 and 72 hours when treated with the high dose. In addition, there was a statistically significant difference in the mean percent of polychromatic erythrocytes in the high dose group at 48 and 72 hours and in the mid dose group at 48 hours. These observations indicate that the test material was toxic to mouse bone marrow at higher concentrations, but did not induce micronuclei formation. |
| **Conclusions** | Under conditions of this assay, the test material is not considered clastogenic in mice up to and including 5.0 g/kg when evaluated up to 72 hours after dose administration. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | "In vivo mammalian bone marrow micronucleus assay: oral gavage method," Exxon Biomedical Sciences, Inc. 1991. |
| **Date last changed** | October, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance**<br>**CAS No.** | Alkenes, C8-10, C9 rich<br>68526-55-6 |
| **Method/Guideline**<br>**Test Type**<br>**GLP**<br>**Year** | EPA OTS 798.5265<br>Ames Assay<br>Yes<br>1991 |
| **Species/strain** | Salmonella typhimurium; TA98; TA100; TA1535; TA1537; TA1538 |
| **Metabolic Activation** | With and without S9 fraction of livers from rats pretreated with Aroclor 1254. |
| **Dose/Conc. Levels** | 10, 32, 100, 320, and 1000 μg/plate |
| **Statistical methods** | The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose. |
| **Remarks on Test Conditions** | |
| Solvent: | DMSO was used for controls; Ethanol was used for the test material |
| Positive Controls: | 2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine |
| Negative Controls: | Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO |
| | To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 μg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 1000 μg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates. |
| | A repeat assay was performed in order to verify the data produced in the initial assay. |
| **Results** | Negative |
| **Remarks** | The test material did not produce any evidence of mutagenicity. Doses were considered positive if test values were equal to or greater than 3X the mean value of the vehicle control. In the initial and repeat assays, neither a positive response nor a dose related increase in revertants was observed for any of the tester strains either in the presence or absence of metabolic activation. All other positive and negative controls responded in a manner consistent with data from previous assays. |
| **Conclusions** | Under conditions of this assay, the test material was not mutagenic for the *Salmonella* tester strains at doses up to and including 1000 μg/plate. |
| **Data Quality** | 1 - Valid without restrictions |
| **Reference:** | Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay; Exxon Biomedical Sciences Inc., 1991. |
| **Date last changed** | November, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_{10}$V-HOF |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Oral |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rats |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 5/sex/dose |
| **Route of administration** | Oral |
| **Vehicle** | NA |
| **Dose/Concentration Levels:** | 5000 mg/kg |
| **Remarks on Test Conditions** | Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose. Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel. |
| **Results** | $LD_{50}$ > 5000 mg/kg |
| **Remarks** | All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area and soft stool in some animals. By Day 12, all animals exhibited no observable abnormalities. Gross postmortem examination revealed no observable abnormalities in any animals. |
| **Conclusions** | Under the conditions of this study, $C_{10}$V-HOF has a low order of acute oral toxicity. |
| **Data Quality** | 1 - Reliable without restrictions. |
| **Reference** | "Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_{10}$U-HOF |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Oral |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rats |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 5/sex/dose |
| **Route of administration** | Oral |
| **Vehicle** | NA |
| **Dose/Concentration Levels:** | 5000 mg/kg |
| **Remarks on Test Conditions** | Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose. Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel. |
| **Results** | $LD_{50}$ > 5000 mg/kg |
| **Remarks** | All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area in some animals. By Day 6, all animals exhibited no observable abnormalities. Gross postmortem examination revealed slight lung discoloration in three animals and no observable abnormalities in the other seven animals. |
| **Conclusions** | Under the conditions of this study, $C_{10}$U-HOF has a low order of acute oral toxicity. |
| **Data Quality** | 1 - Reliable without restrictions. |
| **Reference** | "Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_{10}$V-HOF |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Dermal |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rabbit |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 3/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Dose/Concentration Levels** | 3160 mg/kg |
| **Remarks on Test Conditions** | Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The test material was covered with a gauze patch and secured with tape. To prevent evaporation or ingestion of the test material, the gauze patch was secured to the trunk of the animal with tape and a plastic sleeve. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed. |
| **Results** | $LD_{50}$ > 3160 mg/kg |
| **Remarks** | There were no deaths prior to study termination. Five of six animals displayed an increase in body weight over their initial values, while the remaining animal displayed a slight loss in body weight. Clinical in-life observations were minimal during the study and included soft stool, nasal discharge, anogenital staining, ocular discharge, and alopecia. Gross necropsy revealed discoloration of the kidneys in one animal, salivary glands abnormalities in one animal, and desquamation in two animals. Three of the six test animals exhibited no observable abnormalities at necropsy. The test material produced some dermal irritation, including desquamation. However, by Day 14, only one animal displayed very slight erythema and edema. |
| **Conclusions** | Under the conditions of this study, $C_{10}$V-HOF has a low order acute toxicity by the dermal route of exposure. |
| **Data Quality** | 1 - Reliable without restrictions. |
| **Reference** | "Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 01 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | $C_{10}$U-HOF |
| **CAS No.** | |
| **Method/Guideline** | Other |
| **Type of Study** | Acute Dermal |
| **GLP** | Yes |
| **Year** | 1985 |
| **Species/strain** | Rabbit |
| **Sex** | M/F |
| **No. of animals/sex/dose** | 3/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Dose/Concentration Levels** | 3160 mg/kg |
| **Remarks on Test Conditions** | Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed. |
| **Results** | $LD_{50}$ > 3160 mg/kg |
| **Remarks** | There were no deaths prior to study termination. All animals displayed an increase in body weight over the course of the study. Clinical in-life observations during the study were minimal. One animal that was observed with its collar in its mouth at three consecutive observations intervals exhibited ataxia, nasal discharge, decreased food consumption, emaciation, staining in the anogenital area, a small amount of stool, alopecia, scabs, and maloccluded incisors. This animal had its collar removed for the remainder of the study. Necropsy revealed maloccluded incisors in 1 animal and 3 animals with alopecia. Three of the 6 test animals exhibited no observable abnormalities. Dermal observations included initial moderate-to-severe erythema that diminished in severity by the end of the observation period. Two animals displayed fissuring and all animals displayed atonia and desquamation. |
| **Conclusions** | Under the conditions of this study, $C_{10}$U-HOF has a low order acute toxicity by the dermal route of exposure. |
| **Data Quality** | 1 - Reliable without restrictions |
| **Reference** | "Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc. |
| **Date last changed** | October, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C9-C11 iso, C10 rich |
| **CAS No.** | 68526-85-2 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute oral toxicity |
| **GLP** | Pre-GLP |
| **Year** | 1960 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Male |
| **No. of animals/sex/dose** | 5/dose |
| **Route of administration** | Oral gavage |
| **Vehicle** | Corn oil |
| **Frequency of Treatment** | Single Treatment |
| **Dose/Concentration Levels** | 0.1, 1.0, 10.0, 30.0% volume/volume emulsion in corn oil (Equivalent to 26, 82, 260, 820, 2600, 8200 mg/kg) |
| **Control group and Treatment** | For comparison, untreated animals were necropsied at the end of the study. |
| **Remarks on Test Conditions** | Prior to dosage, food was withheld from the animals for three to four hours. The animals were observed for gross effects and mortality at one, four, and twenty-four hours, and once daily thereafter up until seven days. Gross necropsies were performed at the end of the observation period and samples of liver, kidney, brain, and blood were taken from untreated control animals and from all surviving animals at the 820 and 2600 mg/kg dose levels. |
| **Results** | $LD_{50}$ = 4626 mg/kg |
| **Remarks** | 5/5 animals died within the first four hours following exposure to 8200 mg/kg. Animals in all other dose groups survived until the end of the study. At the one and four-hour intervals, animals in the 260 and 820 mg/kg dose groups were inactive and displayed labored respiration, ataxia, and sprawling of the limbs. At the 24-hour interval, animals had oily fur. After approximately 48-hours after dosing, most animals in these groups returned to normal appearance and behavior. At the 2600 mg/kg dose level, animals exhibited similar symptoms as above but also showed lacrimation and depressed righting and placement reflexes. Animals in this dose group also returned to normal appearance and behavior after 24 hours. At the highest dose, animals initially exhibited labored respiration, ataxia, and sprawling of the limbs, which was followed by a comatose state and death within 4 hours of exposure.<br><br>The surviving animals at the five lower dose levels (26, 82, 260, 820, 2600 mg/kg) had weight gain that was within the normal range. Gross autopsies performed on animals that died (5/5 in 8200 mg/kg group) revealed congested lungs, kidneys, and adrenals, and dark-appearing spleens. No abnormalities were observed in the surviving animals at necropsy. Therefore, a histopathologic analysis was not performed. |
| **Conclusions** | Under the conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of toxicity. |
| **Data Quality** | 2 - Valid with restrictions (Pre-GLP). |
| **Reference** | Esso Research and Engineering (1960). Unpublished report. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C9-C11 iso, C10 rich |
| **CAS No.** | 68526-85-2 |
| **Method/Guideline** | Other |
| **Type of Study** | Acute dermal toxicity |
| **GLP** | Pre-GLP |
| **Year** | 1960 |
| **Species/strain** | Rabbits/Albino |
| **Sex** | Males and Females |
| **No. of animals** | 2/sex/dose |
| **Route of administration** | Dermal |
| **Frequency of Treatment** | Single Dose |
| **Dose/Concentration Levels** | 80, 260, 820, and 2600 mg/kg |
| **Remarks on Test Conditions** | A single application of the test material was given to four groups (2/sex/dose) of four rabbits at doses of 80, 260, 820, and 2600 mg/kg. The material was applied under occlusive dressing to intact abdominal skin. Observations were recorded at one, four and 24 hours; and once daily thereafter for a total of 7 days. Samples of liver, kidney, brain and blood were taken from four untreated control albino rabbits and from each surviving animal at the 820 and 2600 mg/kg dose level. |
| **Results** | The acute dermal LD50 is > 2600 mg/kg |
| **Remarks** | No deaths were observed during this study. Mild to moderate erythema and edema were observed in animals at the three lower dose levels. Marked erythema and edema were observed at the highest dose level. Edema in each animal subsided within 3 days. Erythema in animals at the high dose group diminished in intensity but did not subside completely during the observation period. Autopsies performed following sacrifice revealed no gross pathological findings in any animal. Therefore, a histopathologic analysis was not performed. |
| **Conclusions** | Under conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of acute dermal toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions (Pre-GLP). |
| **Reference** | Esso Research and Engineering (1960). Unpublished report. |
| **Date last changed** | September, 2000 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | Isodecanol |
| **CAS No.** | 25339-17-7 |
| **Method/Guideline** | OECD 414 |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Yes |
| **Year** | 1989 |
| **Species/strain** | Wistar rats |
| **Sex** | Females |
| **No. of animals/sex/dose** | 10/dose |
| **Route of administration** | Oral gavage |
| **Frequency of treatment** | Gestation day 6-15 |
| **Dose/Concentration Levels** | 158, 790, 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) |
| **Statistical methods** | Dunnett's test, Fisher's exact test |
| **Remarks on Test Conditions** | The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 158, 790, or 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings. |
| **Results** | Maternal NOAEL = 158 mg/kg, Fetal NOAEL = 790 mg/kg |
| **Remarks** | At the lowest dose level, no adverse effects were observed in the dams or the fetuses as a result of exposure to the test compound. There were also no differences from controls with respect to the following reproductive parameters: conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, number of viable fetuses, placental weight, and sex distribution of the fetuses.<br><br>Dams of the middle dose group exhibited reduced body weight gain and did not consume as much food as the control animals. Animals in the middle dose group also had an unsteady gait and reddish nasal discharge. No embryo or fetotoxic effects were observed at this dose. In addition, there were no changes in fertility parameters at the middle dose.<br><br>Treatment with the highest dose of isodecanol resulted in statistically significant decreases in food consumption, body weight, and body weight gain in the dams. Three animals in the high dose group were found dead on gestation days 9 and 10. A fourth dam was sacrificed in moribund condition on gestation day 10. All of the dams in the high dose group had clinical symptoms that included nasal discharge, salivation, and signs of CNS depression. |

| | |
|---|---|
| **Results, continued** | At necropsy, the liver was light brown-gray and the mean gravid uterus weight was reduced. The lungs displayed signs of edema and emphysema. There were statistically significant increases in the number of resorptions in the high dose group as well as significantly reduced mean fetal body weight. However, there were no other statistically significant changes in reproductive parameters. Two litters had 2 anedeous fetuses. In addition, there were an increased number of fetuses with skeletal retardations. |
| **Conclusions** | Isodecanol is embryo and fetotoxic at doses that produce overt toxicity in the dam. In the absence of maternal toxicity, isodecanol is not embryo or fetotoxic under the conditions of this study. Furthermore, isodecanol does not alter fertility parameters at doses that are not maternally toxic. |
| **Data Quality** | 2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed. |
| **Reference** | Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245. |
| **Date last changed** | October, 2000 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | 1-Decanol |
| **CAS No.** | -- |
| **Method/Guideline** | Other |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Not specified |
| **Year** | 1989 |
| **Species/strain** | Sprague-Dawley Rats |
| **Sex** | Pregnant females |
| **No. of animals/sex/dose** | 15 dams/treatment |
| **Route of administration** | Inhalation |
| **Frequency of treatment** | 7 hrs/day; Gestation days 1-19 |
| **Dose/Concentration Levels** | 100 $mg/m^3$ (Saturated vapors) |
| **Control group and treatment** | 15 sham-exposed rats |
| **Statistical methods** | MANOVA, ANOVA, Kruskal-Wallis test |
| **Remarks on Test Conditions** | Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Animals had free access to food and water. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 100 $mg/m^3$. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by $CO_2$ asphyxiation, and the uterus and ovaries were removed and examined for corpa lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects. |
| **Results** | NOAEL = 100 $mg/m^3$ |
| **Remarks** | No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups. |

| | |
|---|---|
| **Conclusions** | Under the conditions of this study, exposure of pregnant rats to vapors of 1-Decanol does not induce maternal or fetal toxicity. |
| **Data Quality** | 2 - Reliable with restrictions - Similar to guideline study; only one exposure level. |
| **Reference** | B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) Journal of the American College of Toxicology **9(1)**: 93-97. NIOSH, Division of Biomedical and Behavioral Sciences |
| **Date last changed** | February, 2001 |

## Developmental Toxicity

| | |
|---|---|
| **Test Substance** | C7-9-11 Alcohol<br>The test material consists mainly of linear alcohols and also contains significant amounts of alpha-methyl branched alcohols ranging in carbon chain length from C7 to C11. |
| **CAS No.** | 85566-14-9 |
| **Method/Guideline** | OECD 414 |
| **Type of Study** | Developmental Toxicity |
| **GLP** | Yes |
| **Year** | 1989 |
| **Species/strain** | Rats/Wistar |
| **Sex** | Females |
| **No. of animals/sex/dose** | 10/dose |
| **Route of administration** | Oral gavage |
| **Frequency of treatment** | Gestation day 6-15 |
| **Dose/Concentration Levels** | 144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) |
| **Statistical methods** | Dunnett's test, Fisher's exact test |
| **Remarks on Test Conditions** | The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings. |
| **Results** | Maternal NOAEL ≥ 1,440 mg/kg/day<br>Fetal NOAEL ≥ 1,440 mg/kg/day |
| **Remarks** | No adverse effects were observed at any dose of C7-9-11 Alcohol. This included changes in body weight and food consumption by the dams, reproductive parameters, and signs of fetal toxicity. |
| **Conclusions** | C7-9-11 Alcohol does not produce signs of toxicity in the dam or the fetus. C7-9-11 Alcohol is not embryo or fetotoxic under the conditions of this study. |
| **Data Quality** | 2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed. |
| **Reference** | Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245. |
| **Date last changed** | June, 2001 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C11-14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline** | OECD 401 |
| **Type of Study** | Acute oral toxicity |
| **GLP** | Yes |
| **Year** | 1988 |
| **Species/strain** | Rats/Wistar |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 5/sex/dose |
| **Route of administration** | Oral Gavage |
| **Vehicle** | None |
| **Frequency of Treatment** | Single Dose |
| **Dose/Concentration Levels** | 2000 mg/kg |
| **Control group and Treatment** | None |
| **Remarks on Test Conditions** | The testing procedure used in this study is in accordance with OECD Guidelines 401. After being fasted for 12 to 18 hours, male and female rats were administered a single oral gavage dose of 2,000 mg/kg of the test article. Observations were made four times on day 1; and daily for 14 days. Animals were necropsied at the termination of the study. |
| **Results** | $LD_{50}$ > 2,000 mg/kg. |
| **Remarks** | There were no deaths in males or females. Clinical signs of toxicity that were observed included sedation, diarrhea and dyspnea (males). There were no macroscopic changes observed at necropsy. |
| **Conclusions** | Under the conditions of this study, Alcohols, C11-14 iso, C13 rich has a low order of acute oral toxicity in rats. |
| **Data Quality** | 1 - Valid without restrictions |
| **Reference** | Research and Consulting Co., (1988). Acute Oral Toxicity Study with Alcohols, C11-14 iso, C13 rich in Rats, Unpublished report. |
| **Date last changed** | September, 2000 |

## Genetic Toxicity

| | |
|---|---|
| **Test Substance** | 1-Dodecanol |
| **CAS No.** | 112-53-8 |
| **Method** | Other |
| **Type of Study** | Ames Assay |
| **Test system** | *S. typhimurium, E. coli* |
| **GLP** | Not specified |
| **Year** | 1985 |
| **Species/Strain** | *Salmonella typhimurium* /TA98; TA100; TA1535; TA1537; TA1538; *E. coli* WP2uvrA |
| **Metabolic Activation** | Yes |
| **Concentrations** | 0.01, 0.05, 0.1, 0.5, 1, 5, 10, and 50 ug/plate. |
| **Statistical methods** | Samples run in duplicate. No further details provided. |
| **Remarks on Test Conditions** | 1-dodecanol (90% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls. |
| **Results** | Negative. |
| **Remarks for Results** | There was no evidence of mutagenicity of 1-dodecanol in the presence or absence of metabolic activation in all of the strains tested. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 1-dodecanol samples. |
| **Conclusions** | 1-Dodecanol was not mutagenic in bacteria under the conditions of this study. |
| **Data Quality** | 2- Reliable with restrictions (Similar to OECD 471) |
| **Reference** | H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," *Japanese Journal of Industrial Health*, **27**: 400-419. |
| **Date last changed** | October 3, 2000 |

## Repeat Dose Toxicity

| | |
|---|---|
| **Test Substance** | Alcohols, C11-14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline** | OECD 408 |
| **Type of Study** | Repeated dose 90-day oral toxicity study |
| **GLP** | Yes |
| **Year** | 1986 |
| **Species/strain** | Rats/Sprague-Dawley |
| **Sex** | Males and Females |
| **No. of animals** | 20/sex/dose |
| **Route of administration** | Oral gavage |
| **Frequency of treatment** | Daily, 7 days per week, 14 weeks |
| **Doses** | 0, 100, 500, and 1000 mg/kg/day |
| **Vehicle** | Distilled water |
| **Remarks on Test Conditions** | Rats (20/sex/dose) were administered 0, 100, 500, and 1000 mg/kg/day in a dose volume of 10 ml/kg/day for a total period of 14 weeks. Animals were observed daily for signs of toxicity. Body weight was recorded prior to the initial dose, at the initiation of dosing, and weekly thereafter. At the end of the study full serum chemistry and hematology analyses were performed. A full necropsy was performed on each animal and tissues and organs were preserved. |
| **Results** | NOAEL = 100 mg/kg/day |
| **Remarks** | During the study, there were 5 deaths that could not be attributed to treatment with the test substance. Males in the middle and high dose groups had significantly lower body weights and food consumption than the control animals. However, females did not display any differences in body weight or food consumption.<br><br>Females in the middle and high dose group had statistically significant higher mean platelet counts compared to the control groups. The males did not show any significant differences in mean hematological values. Mean cholesterol increased in high-dose females and glucose decreased in middle-dose females and high-dose animals of both sexes. However, the significance of these findings to treatment with Alcohols, C11-14 iso, C13 rich is not clear.<br><br>Males and females in the middle and high-dose groups had significantly higher liver weights than animals in the control group. High dose males had significantly lower body weights than the control animals. Relative mean brain and testes weights also increased in high-dose males, while relative adrenal weights increased in high-dose females. However, no treatment-related weight or histopathologic changes were observed in the other organs, including female reproductive organs. |
| **Conclusions** | Under the conditions of this study, subchronic oral exposure to the lowest concentration (100 mg/kg/day) of Alcohols, C11-14 iso, C13 rich was not toxic. At higher concentrations, there were some effects on hematologic profile and organ weight, but the significance of these changes is not known. |

| | |
|---|---|
| **Data Quality** | 1 - Valid without restrictions |
| **Reference** | Exxon Biomedical Sciences, Inc. (1986); Subchronic oral gavage study in rats; Unpublished report. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C11-13, C12 rich |
| **CAS No.** | 68526-58-9 |
| **Method/Guideline** | NA |
| **Type of Study** | Oral $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1961 |
| **Species/strain** | Rats /Sprague-Dawley |
| **Sex** | Male |
| **No. of animals/sex/dose** | 5/dose |
| **Route of administration** | Oral gavage |
| **Vehicle** | Corn oil |
| **Frequency of Treatment:** | Single Treatment |
| **Dose/Concentration Levels:** | Either 0.1, 1.0, and 10.0% volume/volume in corn oil or undiluted. (Equivalent to 24.5, 77.4, 245, 774, 2446, and 7440 mg/kg) |
| **Control group and Treatment:** | For comparison, untreated animals were necropsied at the end of the study. |
| **Remarks on Test Conditions** | Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water was available at all times. The animals were observed for gross effects and mortality at 1, 4, and 24 hours and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period. Tissue samples from the 2446 and 7440 mg/kg dose levels were collected for possible further analysis. |
| **Results ($LD_{50}$ or $LC_{50}$):** | $LD_{50}$ > 7740 mg/kg |
| **Remarks** | No mortalities were observed at any of the doses tested. Animals at all dosage levels exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. There were no pathological findings at necropsy. |
| **Conclusions** | Under the conditions of this study, Alkenes, C11-13, C12-rich have a low order of toxicity. |
| **Data Quality** | 1 - Reliable without restrictions, comparable to a guideline study |
| **Reference** | Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C11-13, C12 rich |
| **CAS No.** | 68526-58-9 |
| **Method/Guideline** | NA |
| **Type of Study** | Dermal $LD_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1961 |
| **Species/strain** | Albino rabbits |
| **Sex** | Males and Females |
| **No. of animals/sex/dose** | 2/sex/dose |
| **Route of administration** | Dermal |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single 24-hour exposure |
| **Dose/Concentration Levels:** | 77.4, 245, 774, 2446 mg/kg. |
| **Control group and Treatment:** | NA |
| **Remarks on Test Conditions** | Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. Tissue samples were taken from animals at the 774 and 2446 mg/kg dose levels. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LD_{50}$ > 2446 mg/kg** |
| **Remarks** | No mortalities were observed at any dose tested. One animal in the 245 mgl/kg dose group had diarrhea on the last day of the study and a net loss of weight. The remaining animals exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. One animal in the 1000 µl/kg and two animals in the 2446 mgl/kg dose groups had parasitic infections in the liver. No other abnormalities were observed at necropsy.<br><br>Upon removal of the binders, the exposed skin showed slight erythema. Three of the high dose animals displayed slight edema, which subsided within 48 hours. By 48 hours, low dose animals showed no signs of irritation. Erythema in the high dose animals completely subsided by the third day. By Day 12, all signs of irritation had completely cleared in all of the animals with the exception of slight desquamation in one high dose animal. |
| **Conclusions** | Alkenes, C11-13, C12-rich have a low order of acute dermal toxicity. |
| **Data Quality** | 1 - Reliable without restrictions; comparable to a guideline study. |
| **Reference** | Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961. |
| **Date last changed** | October, 2000 |

## Acute Toxicity

| | |
|---|---|
| **Test Substance** | Alkenes, C11-13, C12 rich |
| **CAS No.** | 68526-58-9 |
| **Method/Guideline** | NA |
| **Type of Study** | Inhalation $LC_{50}$ |
| **GLP** | Pre-GLP |
| **Year** | 1961 |
| **Species/strain** | Mice/Swiss Albino, Rats/Wistar, Guinea pigs/English short hair |
| **Sex** | Males |
| **No. of animals/sex/dose** | 10/species |
| **Route of administration** | Inhalation |
| **Vehicle** | NA |
| **Frequency of Treatment:** | Single Dose |
| **Dose/Concentration Levels:** | 4.4 mg/L for 6 hours (saturated vapors only, no aerosol) |
| **Control group and Treatment:** | Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group. |
| **Remarks on Test Conditions** | Air was bubbled through the test material and into a chamber to give a total flow through the chamber of 35 liters/minute. The theoretical mean chamber concentration (4.4 mg/L) was calculated from the loss of material and airflow through the chamber. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. |
| **Results ($LD_{50}$ or $LC_{50}$):** | **$LC_{50}$ > 4.4 mg/L for 6 hours** |
| **Remarks** | Immediately following initiation of the exposure, all animals exhibited increased motor activity. Lacrimation was observed in rats and guinea pigs beginning at the 90-minute interval. Otherwise, all animals seemed normal in appearance and behavior throughout the study. No abnormalities were observed at necropsy. |
| **Conclusions** | Under conditions of this study, Alkenes, C11-13, C12 rich have a low order of acute inhalation toxicity in rats. |
| **Data Quality** | 2 - Valid with restrictions. No analysis of exposure atmosphere. |
| **Reference** | Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961. |
| **Date last changed** | October, 2000 |

# Olefin Hydroformylation Products Category

## Robust Summaries
## Environmental Fate and Effects

Prepared by:

ExxonMobil Chemical Company

November 19, 2001

## Table of Contents

CAS #68526-58-9; Alkenes C12-14, C13 rich
Manometric Respirometry

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Hexanol branched and linear |
| **CAS No.** | 68526-79-4 |
| **Method/Guideline:** | No Data |
| **Year (guideline):** | No Data |
| **Type (test type):** | Flow Through Acute Fish Toxicity Test |
| **GLP:** | No Data |
| **Year (study performed):** | 1980 |
| **Species:** | Fathead Minnow (*Pimephales promelas*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method: (FT - ME)** | Trimmed Spearman Karber Method |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Treatment solutions were prepared by diluting a 3720mg/L stock solution.<br>Nominal hexanol treatment levels were 41, 68, 113, 189, 315mg/L, which measured 26.7, 49.2, 90.6, 170.0, and 261.5mg/L, respectively.<br>Control/dilution water was EPA Duluth laboratory water.<br>Fifty fish were tested per treatment, divided into two replicates.<br>Treatment volume = 6.3L. Test parameters were as follows: temperature=26.2 Deg C; dissolved oxygen = 6.2mg/L; pH = 7.6; fish age = 28 days old; fish mean wt = 0.117g; fish mean length = 19.7mm; fish loading = 0.464g/L/day.<br>Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA. |
| **Results: (FT - RS)**<br>**Units/Value:** | 96 hour LC50 = 97.7 mg/L (95% CI 89.7 to 106) based upon measured values |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was Gas-Liquid Chromatography. |

| Measured Conc. (mg/L) | Fish Total Mortality (@96 hrs)* |
|---|---|
| Control | 0 |
| 26.7 | 0 |
| 49.2 | 0 |
| 90.6 | 20 |
| 170.0 | 50 |
| 261.5 | 50 |

* 50 fish added at test initiation

| | |
|---|---|
| **Conclusion: (FT - CL)** | |
| **Reliability: (FT - RL)** | (1) Reliable without restriction |
| **Reference: (FT - RE)** | Brooke, L. T. et al. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. I. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA. |
| **Other (source): (FT - SO)** | ExxonMobil Biomedical Sciences, Inc. |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohols C6-8, branched |
| **CAS No.** | 70914-20-4 |
| **Method/Guideline:** | No Data |
| **Year (guideline):** | No Data |
| **Type (test type):** | Flow Through Acute Fish Toxicity Test |
| **GLP:** | No Data |
| **Year (study performed):** | 1985 |
| **Species:** | Fathead Minnow (*Pimephales promelas*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method: (FT - ME)** | Trimmed Spearrman Karber Method |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Treatment solutions were prepared by diluting a 1400mg/L stock solution.<br>Nominal heptanol treatment levels were 12.5, 19.3, 29.7, 45.7, 70.3mg/L, which measured 12.5, 18.1, 28.5, 43.6, and 70.8mg/L, respectively.<br>Control/dilution water was EPA Duluth laboratory water.<br>Twenty fish were tested per treatment. Treatment volume = 2.0L.<br>Test parameters were as follows: temperature=25.6 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 31 days old; fish mean wt = 0.100g; fish mean length = 18.1mm; fish loading = 1.0g/L/day.<br>Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA. |
| **Results: (FT - RS)**<br>**Units/Value:** | 96 hour LC50 = 34.5 mg/L (95% CI 33.1 to 36.0) based upon measured values |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was Gas-Liquid Chromatography. |

| Measured Conc. (mg/L) | Fish Total Mortality (@96 hrs)* |
|---|---|
| Control | 0 |
| 12.5 | 0 |
| 18.1 | 1 |
| 28.5 | 0 |
| 43.6 | 20 |
| 70.8 | 20 |

* 20 fish added at test initiation

| | |
|---|---|
| **Conclusion: (FT - CL)** | |
| **Reliability: (FT - RL)** | (1) Reliable without restriction |
| **Reference: (FT - RE)** | Geiger, D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. III. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA. |
| **Other (source): (FT - SO)** | ExxonMobil Biomedical Sciences, Inc. |

# Invertebrate Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C6-8, branched |
| **CAS No.** | 70914-20-4 |
| **Method/Guideline:** | Concept rules of the Dutch Standardization Institute (Adema, 1978) |
| **Type (test type):** | Daphnid Acute Toxicity Test |
| **GLP:** | No Data |
| **Year (study performed):** | 1978 |
| **Species:** | Water Flea (*Daphnia magna*) |
| **Analytical Monitoring:** | No |
| **Exposure Period:** | 48 hour |
| **Statistical Method:** | No Data |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Tests using 15 different chemicals, including n-Heptanol, were performed at two different laboratories. Lab I was the National Institute of Public Health, Bilthoven, The Netherlands; Lab II was the Central Laboratory, T.N.O., Delft, The Netherlands. The tests were conducted using standardized tests methods proposed by the Dutch Standardization Institute (Adema, 1978). The tests were conducted in duplicate to determine the reprodicibility of the results.<br>Organisms were supplied by in-house cultures. Age = <24 hours old. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | 48-hour EC50 = 63 mg/L, based upon nominal concentrations of the test chemicals. |
| **Conclusion:** | Test substance is considered to have moderate acute toxicity |
| **Reliability:** | Code 2, Reliable with Restrictions |
| **Reference:** | Canton, J.H. and D.M.M. Adema. 1978. Reproducibility of Short-term and Reproduction Toxicity Experiments with *Daphnia magna* and Comparison of the Sensitivity of *Daphnia magna* with *Daphnia pulex* and *Daphnia cucullata* in Short-term Experiments. *Hydrobiologia*, **59**:2, pp. 135-140. |

| | |
|---|---|
| **Other (reference)** | Adema, D.M.M. 1978. Daphnia magna as Test Organism in Acute and Chronic Toxicity Experiments. *Hydrobiologia*, **59**:2, pp. 125-134. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alkenes, C6 Rich |
| **CAS No.** | 68526-52-3 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Trimmed Spearman-Karber Method (Hamilton, M.A. et al. 1977. Trimmed Spearman-Karber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.) |

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of ≤10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 5 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 6.25, 12.5, 25, 50, and 100 mg/L, which measured 2.9, 6.6, 13.4, 16.9, and 44.0 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Test temperature was 16C (sd = 0.04). Lighting was 623 to 629 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 7.7 to 9.6 mg/L for "new" solutions and 4.5 to 7.5 mg/L for "old" solutions. The pH ranged from 8.2 to 8.5 for "new" solutions and 7.2 to 7.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

**Results:**

**Units/Value:**

LC50 = 6.6mg/L (CI 5.4 to 8.0), based upon measured concentrations of mean of old and new samples.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-FID

LL50 = 12.8mg/L (CI 10.7 to 15.3), based upon nominal loading levels.

| Loading Rate (mg/L) | Measured Conc. (mg/L) | Fish Total Mortality (@96 hrs)* |
|---|---|---|
| Control | Control | 0 |
| 6.25 | 2.9 | 0 |
| 12.5 | 6.6 | 7 |
| 25 | 13.4 | 15 |
| 50 | 16.9 | 15 |
| 100 | 44.0 | 15 |

* 15 fish added at test initiation

**Conclusion:**

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119058.

**Other (source):** American Chemistry Council, Higher Olefins Panel

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohols C7-9, branched |
| **CAS No.** | 68526-83-0 |
| **Method/Guideline:** | No Data |
| **Year (guideline):** | No Data |
| **Type (test type):** | Flow Through Acute Fish Toxicity Test |
| **GLP:** | No Data |
| **Year (study performed):** | 1986 |
| **Species:** | Fathead Minnow (*Pimephales promelas*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method: (FT - ME)** | Trimmed Spearman Karber Method |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Treatment solutions were prepared by diluting a 275mg/L stock solution.<br>Nominal octanol treatment levels were 8.6, 10.8, 13.5, 16.9, 21.1mg/L, which measured 8.8, 10.7, 12.7, 16.5, and 20.4mg/L, respectively.<br>Control/dilution water was EPA Duluth laboratory water.<br>Twenty fish were tested per treatment. Treatment volume = 2.0L.<br>Test parameters were as follows: temperature=25.3 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 28 days old; fish mean wt = 0.075g; fish mean length = 16.5mm; fish loading = 0.75g/L/day.<br>Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA. |
| **Results: (FT - RS)**<br>**Units/Value:** | 96 hour LC50 = 14.0 mg/L (95% CI 13.6 to 14.5) based upon measured values |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was Gas-Liquid Chromatography. |

| Measured Conc. (mg/L) | Fish Total Mortality (@96 hrs)* |
|---|---|
| Control | 0 |
| 8.8 | 0 |
| 10.7 | 1 |
| 12.7 | 2 |
| 16.5 | 20 |
| 20.4 | 20 |

* 20 fish added at test initiation

| | |
|---|---|
| **Conclusion: (FT - CL)** | |
| **Reliability: (FT - RL)** | (1) Reliable without restriction |
| **Reference: (FT - RE)** | Geiger, D.L. et al. 1988. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. IV. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA. |
| **Other (source): (FT - SO)** | ExxonMobil Biomedical Sciences, Inc. |

# Invertebrate Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C7 - 9 branched |
| **CAS No.** | 68526-83-0 |
| **Method/Guideline:** | US EPA 660/3-75-009 |
| **Type (test type):** | Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians |
| **GLP:** | Unknown |
| **Year (study performed):** | 1980 |
| **Species:** | Water Flea (*Daphnia magna* Straus) |
| **Analytical Monitoring:** | No |
| **Exposure Period:** | 48 hour |
| **Statistical Method:** | Spearman-Karber (Finney, D.J., 1971) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Individual treatments were prepared by adding varying amounts of test material directly to 250 mL of dilution water in glass beakers. Nominal test concentrations were 10, 18, 32, 56, 100 and 180 mg/L. Four replicates were prepared for each treatment and control. Five daphnids per replicate chamber. Test placed in a temperature-controlled waterbath at 20.5 to 21.0 Deg. C. The test was performed under static conditions.<br><br>Lighting was 16 hours light : 8 hours dark. Dissolved oxygen ranged from 8.6 to 9.6 mg/L during the study. The pH was ranged from 7.8 to 8.4 during the study. Dilution water hardness was 240 mg/L as $CaCO_3$, alkalinity was 145 mg/L as $CaCO_3$, and conductivity was 600 µmhos/cm.<br><br>Organisms were supplied by in-house cultures. Age = <20 hours old. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | 48-hour LC50 = 31.8 mg/L (CI 26.5 - 38.2) as Total Carbon, based upon nominal concentrations. |

**Results continued**

| Nominal Conc. | % Mortality @ 48 hr. |
|---|---|
| Control | 0 |
| 10 mg/L | 10 |
| 18 mg/L | 20 |
| 32 mg/L | 25 |
| 56 mg/L | 95 |
| 100 mg/L | 100 |
| 180 mg/L | 100 |

**Conclusion:** Test substance is considered to have moderate acute toxicity.

**Reliability:** Code 2, Reliable with Restrictions

Analytical verification not performed, quality assurance unknown.

**Reference:** Union Carbide Corp. (1980). "The Acute Toxicity of MRD-80-4 to the Water Flea (*Daphnia magna* Straus). Unpublished report.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Biodegradation

**Test Substance:** Alcohols C7-9, branched

**CAS No.** 68526-83-0

**Method/Guideline:** OECD 301F, 1992

**Type (test type):** Manometric Respirometry Test

**GLP:** Yes

**Year (study performed):** 1997

**Inoculum:** Domestic activated sludge

**Exposure Period:** 28 days

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 51 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

**Results:**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 82% degradation of the test material was observed. 10% biodegradation was achieved on day 3.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 84.7, 77.1, 84.0 | 82.0 |
| Na Benzoate | 91.3, 81.3 | 86.3 |

* replicate data

**Conclusion:** Test substance is considered readily biodegradable.

**Reliability:** Code 1, Reliable without Restrictions

| | |
|---|---|
| **Reference:** | Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114794A.. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Partition Coefficient

| | |
|---|---|
| **Test Substance:** | Alcohol C7-9, branched |
| **CAS No.** | 68526-83-0 |
| **Method/Guideline:** | OECD 117 |
| **Year (guideline):** | 1989 |
| **Type (test type):** | N-Octanol/Water Partition Coefficient (HPLC method) |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Temperature:** | ~30 Deg C |
| **Log Pow Value:** | 2.9 - 3.4 |
| **Test Conditions:**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.<br><br>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.<br><br>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.<br><br>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | The test substance eluted as several groups. The three major components C7, C8, C9 alcohols had Log Pow values of 2.9, 3.0, and 3.4 respectively.<br><br>The retention time for the 3 major components were 5.72, 6.03, and 7.28 minutes.<br><br>All values were measured using High Performance Liquid Chromatography (HPLC). |
| **Conclusion:** | |

| | |
|---|---|
| **Reliability:** | (1) Reliable without restriction |
| **Reference:** | Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Biodegradation

| | |
|---|---|
| **Test Substance:** | Alkenes, C7-9, C8 Rich |
| **CAS No.** | 68526-54-5 |
| **Method/Guideline:** | OECD 301F, 1993 |
| **Type (test type):** | Manometric Respirometry Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Inoculum:** | Domestic activated sludge |
| **Exposure Period:** | 28 days |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).<br>Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.<br>Test material was tested in triplicate, controls and blanks were tested in duplicate.<br>Test material concentration was approximately 32 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.<br>Test temperature was 22 +/- 1 Deg C.<br><br>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Approximately 29% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on day 17.<br>By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted.<br>Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material. |

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 44.1, 28.6, 15.0 | 29.2 |
| Na Benzoate | 98.9,95.5 | 97.2 |

* replicate data

| | |
|---|---|
| **Conclusion:** | |
| **Reliability:** | Code 1, Reliable without Restrictions |

| | |
|---|---|
| **Reference:** | Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 119194A.. |
| **Other (source):** | American Chemistry Council, Higher Olefins Panel |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alkenes, C7-9, C8 Rich |
| **CAS No.** | 68526-54-5 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Trimmed Spearman-Karber Method (Hamilton, M.A. et al. 1977. Trimmed Spearman-Karber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.) |

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of ≤10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 2.6, 4.3, 7.2, 12, and 20 mg/L, which measured 0.2, 0.4, 0.7, 1.2, and 2.5 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Test temperature was 15C (sd = 0.09). Lighting was 578 to 580 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.5 to 10.2 mg/L for "new" solutions and 6.5 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.0 to 8.4 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test

initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

**Results:**

**Units/Value:**

LC50 = 0.87mg/L (CI 0.79 to 0.96), based upon measured concentrations of mean of old and new samples.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-FID

LL50 = 8.9mg/L (CI 9.9 to 13.3), based upon nominal loading levels.

| Loading Rate (mg/L) | Measured Conc. (mg/L) | Fish Total Mortality (@96 hrs)* |
|---|---|---|
| Control | Control | 0 |
| 2.6 | 0.2 | 0 |
| 4.3 | 0.4 | 0 |
| 7.2 | 0.7 | 1 |
| 12 | 1.2 | 12 |
| 20 | 2.5 | 12 |

* 12 fish added at test initiation

**Conclusion:**

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119158.

**Other (source):** American Chemistry Council, Higher Olefins Panel

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C8 - 10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Bionomial Method |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.<br><br>Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.0 mg/L and from 4.8 to 6.3 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.5 during the study. Fish were not fed during the study.<br><br>Fish Mean Wt.= 0.361g. Mean Total length = 3.8cm, Test Loading = 0.40 g of fish/L. |
| **Results:**<br><br>**Units/Value:** | LC50 = 10.1mg/L (CI 7.3 to 14.1), based upon measured concentrations of mean of old and new samples. |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was GC-FID<br><br>LL50 = 11.2 mg/L (CI 7.5 to 16.6), based upon nominal loading levels. |

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 96 hr. |
|---|---|---|
| Control | Below detection | 0 |
| 0.7 mg/L | 1.7 mg/L | 0 |
| 1.5 mg/L | 1.9 mg/L | 0 |
| 3.3 mg/L | 3.9 mg/L | 0 |
| 7.5 mg/L | 7.3 mg/L | 0 |
| 16.6 mg/L | 14.1 mg/L | 100 |

Dissolved oxygen levels dropped below 60% of saturation in some of the treatments on Days 1 through 4 of the test. Since no mortality occurred in these treatments, the deviations are not believed to have affected the outcome of the study.

**Conclusion:** Test substance is considered to have moderate acute toxicity

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114858.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Invertebrate Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C8-10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline:** | OECD 202 Daphnia sp. Acute Immobilization Test |
| **Type (test type):** | Daphnid Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1996 |
| **Species:** | Water Flea (*Daphnia magna*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 48 hour |
| **Statistical Method:** | Probit procedure of SAS (Finney, 1971) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 25 hours at a vortex of </= 20% of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration.<br><br>Test temperature was 21.4 Deg C., Lighting was 16 hours light : 8 hours dark with 638 to 639 Lux during full daylight periods. Dissolved oxygen ranged from 7.3 to 8.2 mg/L during the study. The pH was ranged from 7.7 to 8.4 during the study.<br><br>Organisms were supplied by in-house cultures. Age = <24 hours old, from 13 and 16-day old parents. |
| **Results:**<br><br>**Units/Value:** | 48-hour EC50 = 4.9 mg/L (CI 4.5 - 5.4), based upon measured concentrations of mean of old and new samples. |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was Total Organic Carbon (TOC). |

| | Nominal Conc. | Measured Conc. | % Immobilization @ 24 hr. |
|---|---|---|---|
| **Results continued** | Control | 0 | 0 |
| | 1.56 mg/L | 0.80 mg/L | 0 |
| | 3.12 mg/L | 1.82 mg/L | 0 |
| | 6.25 mg/L | 3.05 mg/L | 0 |
| | 12.5 mg/L | 4.39 mg/L | 40 |
| | 25.0 mg/L | 6.14 mg/L | 85 |

**Conclusion:** Test substance is considered to have moderate acute toxicity

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Acute Toxicity for Daphnia, 149542.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Algal Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C8-10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline:** | 7-Day Cell Multiplication Inhibition Test |
| **Type (test type):** | Static Toxicity Test |
| **GLP:** | No Data |
| **Year (study performed):** | No Data |
| **Species/Strain:** | Green Alga (*Scenedesmus quadricauda*) |
| **Analytical Monitoring:** | No |
| **Exposure Period:** | 7 days |
| **Statistical Method:** | None applied. The toxicity threshold (TT) was determined graphically by plotting the highest non-toxic concentration versus its mean extinction value against the lowest toxic concentration versus its mean extinction value and calculating the toxicant concentration at 3% below the no effect level. |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.** | Treatment solutions were prepared by diluting a stock isooctanol solution. Testing was conducted in metal capped, 300 ml Erlenmeyer flasks containing 50 ml of treatment solution. Treatment solutions contained isooctanol, cells, double distilled water, and a sterile, defined nutrient medium. The control solution contained nutrient medium, to which sterile double distilled water was added. Growth inhibition measurements were only determined on day 7.<br><br>Cell growth was determined by using a turbidimetric procedure that measured primary light extinction (monochromatic radiation at 578 nm) through a cell suspension of 10 mm thickness. |
| **Results:**<br>**Units/Value:**<br>**Measurement (cells/growth)**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | 7-day TT (toxicity threshold) for growth = 8.5 mg/L based on nominal values<br><br>The TT value for growth is calculated by identifying the treatment level that is greater or equal to 3% below the treatment level that did not exhibit toxic effects as measured by the extinction of primary light of monochromatic radiation at 578 nm. |
| **Conclusion:** | |

| | |
|---|---|
| **Reliability:** | (2) Reliable with restrictions<br><br>Although a non-standardized method was described in the article, data were not provided on the test parameters, replication, or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2. |
| **Reference:** | Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Research. 14:231-241. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Partition Coefficient

| | |
|---|---|
| **Test Substance:** | Alcohol C8-10 iso, C9 rich |
| **CAS No.** | 68526-84-1 |
| **Method/Guideline:** | OECD 117 |
| **Year (guideline):** | 1989 |
| **Type (test type):** | N-Octanol/Water Partition Coefficient (HPLC method) |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Temperature:** | ~30 Deg C |
| **Log Pow Value:** | 3.4 - 3.9 |
| **Test Conditions:**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.<br><br>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.<br><br>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.<br><br>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | The test substance eluted as several groups. The three major components C8, C9, C10 alcohols had Log Pow values of 3.4, 3.8, and 3.9 respectively.<br><br>The retention time for the 3 major components were 6.91, 8.42, and 8.96 minutes.<br><br>All values were measured using High Performance Liquid Chromatography (HPLC). |
| **Conclusion:** | |

| | |
|---|---|
| **Reliability:** | (1) Reliable without restriction |
| **Reference:** | Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C9 - 11 iso, C10 rich |
| **CAS No.** | 68526-85-2 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Probit procedure of SAS (Finney, 1971) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The carboys were covered with an opaque covering to prevent photochemical degradation of the soluble components. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.<br><br>Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 569 to 572 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.9 mg/L and from 5.7 to 7.6 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 8.5 during the study. Fish were not fed during the study.<br><br>Fish Mean Wt.= 0.185g. Mean Total length = 3.0cm, Test Loading = 0.21 g of fish/L. |
| **Results:**<br>**Units/Value:** | LC50 = 3.1mg/L (CI 2.4 to 4.0), based upon measured concentrations of mean of old and new samples. |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was GC-FID<br><br>LL50 = 3.0 mg/L (Could not calculate CI), based upon nominal loading levels. |

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 96 hr. |
|---|---|---|
| Control | Below detection | 7 |
| 1.2 mg/L | 1.2 mg/L | 13 |
| 2.5 mg/L | 2.4 mg/L | 13 |
| 5 mg/L | 5.2 mg/L | 100 |
| 10 mg/L | 9.9 mg/L | 100 |
| 20 mg/L | 19.5 mg/L | 100 |

Dissolved oxygen levels dropped below 60% (57%)of saturation in the 2.4 mg/L treatment on Days 3 and 4 of the test. Since only 13% mortality occurred at this level, and the solutions were renewed daily, this drop in DO did not affect the outcome of the study.

**Conclusion:** Test substance is considered to have moderate acute toxicity

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114958.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Biodegradation

**Test Substance:** Alcohol C9 - 11 iso, C10 rich

**CAS No.** 68526-85-2

**Method/Guideline:** OECD 301F, 1992

**Type (test type):** Manometric Respirometry Test

**GLP:** Yes

**Year (study performed):** 1997

**Inoculum:** Domestic activated sludge

**Exposure Period:** 28 days

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

**Results:**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 71.1% degradation of the test material was observed. 10% biodegradation was achieved on day 4.
By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 74.0, 72.6, 66.5 | 71.1 |
| Na Benzoate | 91.3, 81.3 | 86.3 |

* replicate data

**Conclusion:** Test substance is considered readily biodegradable.

**Reliability:** Code 1, Reliable without Restrictions

| | |
|---|---|
| **Reference:** | Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114994A.. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Partition Coefficient

| | |
|---|---|
| **Test Substance:** | Alcohol C9 - 11 iso, C10 rich |
| **CAS No.** | 68526-85-2 |
| **Method/Guideline:** | OECD 117 |
| **Year (guideline):** | 1989 |
| **Type (test type):** | N-Octanol/Water Partition Coefficient (HPLC method) |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Temperature:** | ~30 Deg C |
| **Log Pow Value:** | 3.8 |
| **Test Conditions:**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.<br><br>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.<br><br>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.<br><br>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported. |
| **Results:**<br>**Units/Value:** | The test substance eluted as several groups. The two major components C9, C10 alcohols had Log Pow values of 3.8. |
| • **Note: Deviations from protocol or guideline, analytical method.** | The retention time for the 2 major components were 8.37, and 8.74 minutes.<br><br>All values were measured using High Performance Liquid Chromatography (HPLC). |
| **Conclusion:** | |

| | |
|---|---|
| **Reliability:** | (1) Reliable without restriction |
| **Reference:** | Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C10 - 12, C11 rich |
| **CAS No.** | 90604-37-8 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Probit procedure of SAS (Finney, 1971) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.<br><br>Test temperature was 15 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 10.0 mg/L and from 4.8 to 6.4 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.6 during the study. Fish were not fed during the study.<br><br>Fish Mean Wt.= 0.365g. Mean Total length = 3.6cm, Test Loading = 0.40 g of fish/L. |
| **Results:**<br>**Units/Value:** | LC50 = 1.8 mg/L (CI 1.4 to 2.5), based upon measured concentrations of mean of old and new samples. |
| • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Analytical method used was GC-MSD<br><br>LL50 = 2.1 mg/L (CI 1.7 to 2.8), based upon nominal loading levels. |

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 96 hr. |
|---|---|---|
| Control | Below detection | 0 |
| 0.3 mg/L | 0.48 mg/L | 13 |
| 0.5 mg/L | 0.52 mg/L | 0 |
| 1.4 mg/L | 1.1 mg/L | 0 |
| 3.5 mg/L | 3.1 mg/L | 100 |
| 8.8 mg/L | 7.2 mg/L | 100 |

Dissolved oxygen levels dropped below 60% (40-60%) of saturation in some of the treatments on Days 1 through 4 of the test. Based on mortality observations, these deviations are not believed to have affected the outcome of the study.

**Conclusion:** Test substance is considered to have moderate acute toxicity

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118458.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alkenes, C9-11, C10 Rich |
| **CAS No.** | 68526-56-7 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Trimmed Spearman-Karber Method (Hamilton, M.A. et al. 1977. Trimmed Spearman-Karber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.) |

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of <10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 0.2, 0.4, 1.2, 3.5, and 10 mg/L, which measured 0.01, 0.03, 0.06, 0.08, and 2.6 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.03 mg/L.

Test temperature was 16C (sd = 0.2). Lighting was 445 to 555 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.7 to 9.9 mg/L for "new" solutions and 7.2 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.3 to 8.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.175 g; mean total length at test termination = 3.0 cm; test loading = 0.19 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

**Results:**

**Units/Value:**

96-hour LL50 = 4.8 mg/L (95% CI 3.8 to 6.0 mg/L) based upon loading rates.
96-hour LC50 = 0.12 mg/L (95% CI 0.11 to 0.14 mg/L) based upon measured values of old and new solutions.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 96 hr.* |
|---|---|---|
| Control | Control | 0 |
| 0.2 mg/L | 0.01 mg/L | 0 |
| 0.4 mg/L | 0.03 mg/L | 0 |
| 1.2 mg/L | 0.06 mg/L | 0 |
| 3.5 mg/L | 0.08 mg/L | 3 |
| 10.0 mg/L | 0.26 mg/L | 15** |

* 15 fish added at test initiation

** 1 mortality not test related

**Conclusion:**

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119258.

**Other (source):** American Chemistry Council, Higher Olefins Panel

# Biodegradation

**Test Substance:** Alkenes, C9-11, C10 Rich

**CAS No.** 68526-56-7

**Method/Guideline:** OECD 301F, 1993

**Type (test type):** Manometric Respirometry Test

**GLP:** Yes

**Year (study performed):** 1995

**Inoculum:** Domestic activated sludge

**Exposure Period:** 28 days

**Test Conditions:**

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.
Test material was tested in triplicate, controls and blanks were tested in duplicate.
Test material concentration was approximately 42 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.
Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

**Results:**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was not readily biodegradable. Approximately 21% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on Day 17. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 20.9, 19.9, 22.6 | 21.1 |
| Na Benzoate | 98.9,95.5 | 97.2 |

* replicate data

**Conclusion:** Test substance is considered not readily biodegradable.

**Reliability:** Code 1, Reliable without Restrictions

| | |
|---|---|
| **Reference:** | Exxon Biomedical Sciences, Inc. 1997. Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119294A. |
| **Other (source):** | American Chemistry Council, Higher Olefins Panel |

# Fish Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C11 - 14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline:** | OECD 203 Fish Acute Toxicity Test |
| **Type (test type):** | Fish Acute Toxicity Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Species:** | Rainbow Trout (*Oncorhynchus mykiss*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 96 hour |
| **Statistical Method:** | Spearman-Karber Method (Hamilton, et al, 1977) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of </= 10% of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.<br><br>Test temperature was 13.8 Deg C., Lighting was 16 hours light : 8 hours dark with 551 to 736 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.3 to 9.2 mg/L and from 6.6 to 8.8 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.2 during the study. Fish were not fed during the study.<br><br>Fish Mean Wt.= 0.131g. Mean Total length = 2.7cm, Test Loading = 0.15 g of fish/L. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | LC50 = 0.42 mg/L (CI 0.37 to 0.48), based upon measured concentrations of mean of old and new samples.<br><br>Analytical method used was GC-MSD<br><br>LL50 = 0.64 mg/L (CI 0.57 to 0.73), based upon nominal loading levels. |

**survival.**

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 96 hr. |
|---|---|---|
| Control | Below detection | 0 |
| 0.25 mg/L | 0.17 mg/L | 0 |
| 0.5 mg/L | 0.32 mg/L | 13 |
| 1.0 mg/L | 0.67 mg/L | 100 |
| 2.0 mg/L | 0.94 mg/L | 100 |
| 5.0 mg/L | 0.93 mg/L | 100 |

**Conclusion:** Test substance is considered to have high acute toxicity

**Reliability:** Code 1, Reliable without Restrictions

**Reference:** Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118358A.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Invertebrate Acute Toxicity

| | |
|---|---|
| **Test Substance:** | Alcohol C11 - 14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline:** | US EPA TSCA 797.1300 |
| **Type (test type):** | Daphnid Acute Toxicity Test |
| **GLP:** | Unknown |
| **Year (study performed):** | 1986 |
| **Species:** | Water Flea (*Daphnia magna*) |
| **Analytical Monitoring:** | Yes |
| **Exposure Period:** | 48 hour |
| **Statistical Method:** | Probit procedure based on Litchfield-Wilcoxon (1949) |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | The water soluble fraction (WSF) was prepared by combining the test substance with dilution water at a ratio of 1:150. The solutions were mixed for 96 hours and allowed to settle for 1 hour prior to use as the 100% WSF stock solution. Test solutions were prepared by diluting the 100% WSF stock. Two replicates of 250 mL in 400 mL autoclaved glass beakers were prepared at each treatment level. Ten daphnids per replicate chamber. Test chambers were covered with glass and placed in a temperature-controlled waterbath. The test was performed under static conditions.<br><br>Test temperature was 20.8 Deg C., Lighting was 16 hours light : 8 hours dark with 57.5 to 67.3 footcandles during full daylight periods. Dissolved oxygen ranged from 8.1 to 9.1 mg/L during the study. The pH was ranged from 7.8 to 8.2 during the study. Dilution water hardness was 130 mg/L as $CaCO_3$.<br><br>Organisms were supplied by in-house cultures. Age = <24 hours old from 19-day old parents. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | 48-hour LC50 = 0.71 mg/L (CI 0.59 - 0.85) as Total Carbon, based upon mean measured concentrations of Day 0 and Day 2 samples. 48-hour LC50 value equivalent to 16.7% WSF.<br><br>Analytical method used was Total Carbon |

**Results continued**

| Nominal Conc. | Measured Conc. | % Mortality @ 48 hr. |
|---|---|---|
| Control | - | 0 |
| 6.25% WSF | 0.28 mg/L | 0 |
| 12.5% WSF | 0.58 mg/L | 30 |
| 25% WSF | 1.03 mg/L | 85 |
| 50% WSF | 1.85 mg/L | 100 |
| 100% WSF | 4.17 mg/L | 100 |

**Conclusion:** Test substance is considered to have high acute toxicity.

**Reliability:** Code 2, Reliable with Restrictions

Analytical verification not test substance specific, quality assurance unknown.

**Reference:** Exxon Biomedical Sciences, Inc. Static Acute Daphnia Toxicity Test, 269342.

**Other (source):** ExxonMobil Biomedical Sciences, Inc.

# Biodegradation

| | |
|---|---|
| **Test Substance:** | Alcohol C11 - 14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline:** | OECD 301F, 1992 |
| **Type (test type):** | Manometric Respirometry Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Inoculum:** | Domestic activated sludge |
| **Exposure Period:** | 28 days |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).<br>Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.<br>Test material was tested in triplicate, controls and blanks were tested in duplicate.<br>Test material concentration was approximately 57 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.<br>Test temperature was 22 +/- 1 Deg C.<br><br>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Test material was not readily biodegradable. Half-life was reached by day 25. By day 28, 58.1% degradation of the test material was observed. 10% biodegradation was achieved on day 7.<br>By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.<br>Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material. |

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 60.1, 60.7, 53.7 | 58.1 |
| Na Benzoate | 87.1, 85.4 | 86.2 |

* replicate data

| | |
|---|---|
| **Conclusion:** | Test substance is considered not readily biodegradable. |
| **Reliability:** | Code 1, Reliable without Restrictions |

| | |
|---|---|
| **Reference:** | Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 180294A.. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Partition Coefficient

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|---|---|
| **Test Substance:** | Alcohol C11 - 14 iso, C13 rich |
| **CAS No.** | 68526-86-3 |
| **Method/Guideline:** | OECD 117 |
| **Year (guideline):** | 1989 |
| **Type (test type):** | N-Octanol/Water Partition Coefficient (HPLC method) |
| **GLP:** | Yes |
| **Year (study performed):** | 1998 |
| **Temperature:** | ~30 Deg C |
| **Log Pow Value:** | 4.2 - 5.0 |
| **Test Conditions:**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.<br><br>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.<br><br>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.<br><br>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | The test substance eluted as several groups. The five major components C9, C10, C11, C12, C13 alcohols had Log Pow values of 4.2, 4.4, 4.5, 4.7, and 5.0 respectively.<br><br>The retention time for the 4 major components were 11.04, 12.02, 13.53, 14.69, and 18.40 minutes.<br><br>All values were measured using High Performance Liquid Chromatography (HPLC). |
| **Conclusion:** | |

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| **Reliability:** | (1) Reliable without restriction |
| **Reference:** | Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D. |
| **Other (source):** | ExxonMobil Biomedical Sciences, Inc. |

# Biodegradation

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| **Test Substance:** | Alkenes, C12-14, C13 Rich |
| **CAS No.** | 68526-58-9 |
| **Method/Guideline:** | OECD 301F, 1993 |
| **Type (test type):** | Manometric Respirometry Test |
| **GLP:** | Yes |
| **Year (study performed):** | 1995 |
| **Inoculum:** | Domestic activated sludge |
| **Exposure Period:** | 28 days |
| **Test Conditions:**<br>• **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.** | Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).<br>Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.<br>Test material was tested in triplicate, controls and blanks were tested in duplicate.<br>Test material concentration was approximately 45 mg/L. Sodium benzoate (positive control) concentration was 50mg/L.<br>Test temperature was 22 +/- 1 Deg C.<br>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates. |
| **Results:**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.** | Test material was not readily biodegradable. Approximately 8% biodegradation of the test material was measured on day 28. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.<br>Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material. |

| Sample | % Degradation* (day 28) | Mean % Degradation (day 28) |
|---|---|---|
| Test Material | 6.28, 8.26, 8.35 | 7.63 |
| Na Benzoate | 88.2, 86.5 | 87.4 |

* replicate data

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| **Conclusion:** | Test substance is considered not readily biodegradable. |
| **Reliability:** | Code 1, Reliable without Restrictions |

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| **Reference:** | Exxon Biomedical Sciences, Inc. 1997. Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119394A. |
| **Other (source):** | American Chemistry Council, Higher Olefins Panel |